PROJECTION-BASED MODEL ORDER REDUCTION AND HYPERREDUCTION OF TURBULENT FLOW MODELS

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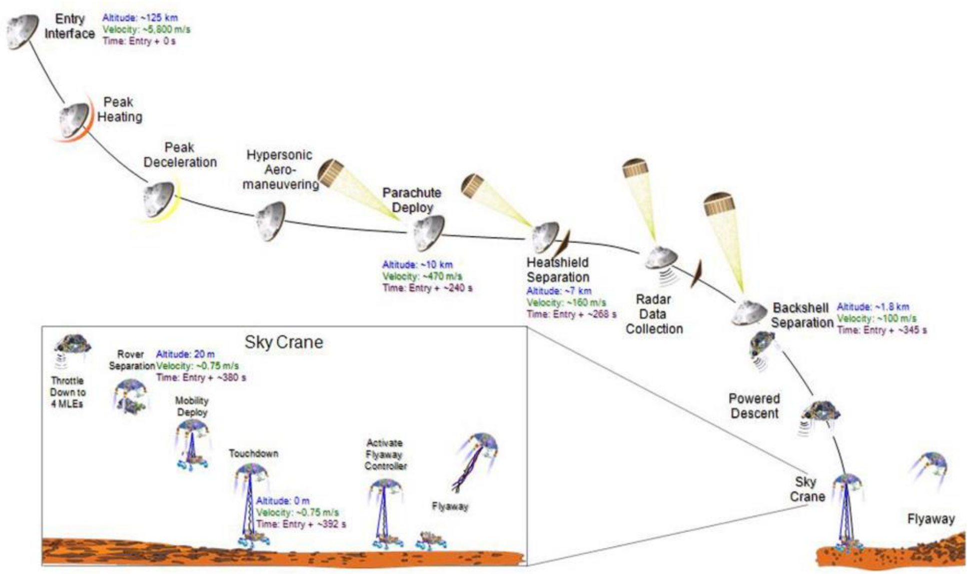
Stanford

- Physics-based simulation for increasingly complex engineered systems
  - Advances in modeling, numerical algorithms, and computational resources have enabled high-fidelity simulation of realistic, large-scale problems

- A concrete example: Curiosity's "Seven Minutes of Terror" (NASA JPL, 2012)



SIMULATION-BASED ENGINEERING SCIENCE

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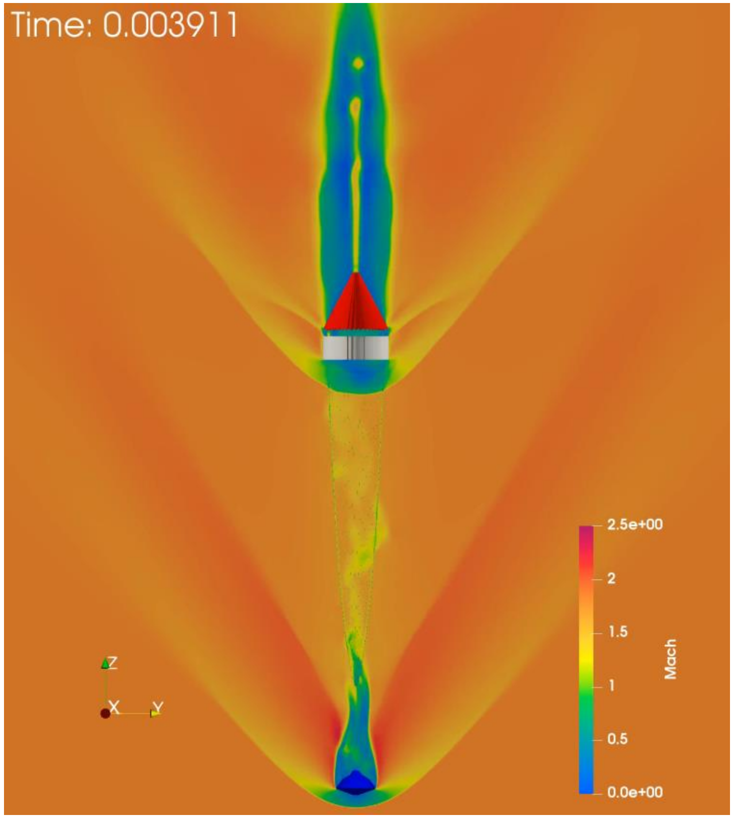


Courtesy of D. Z. Huang

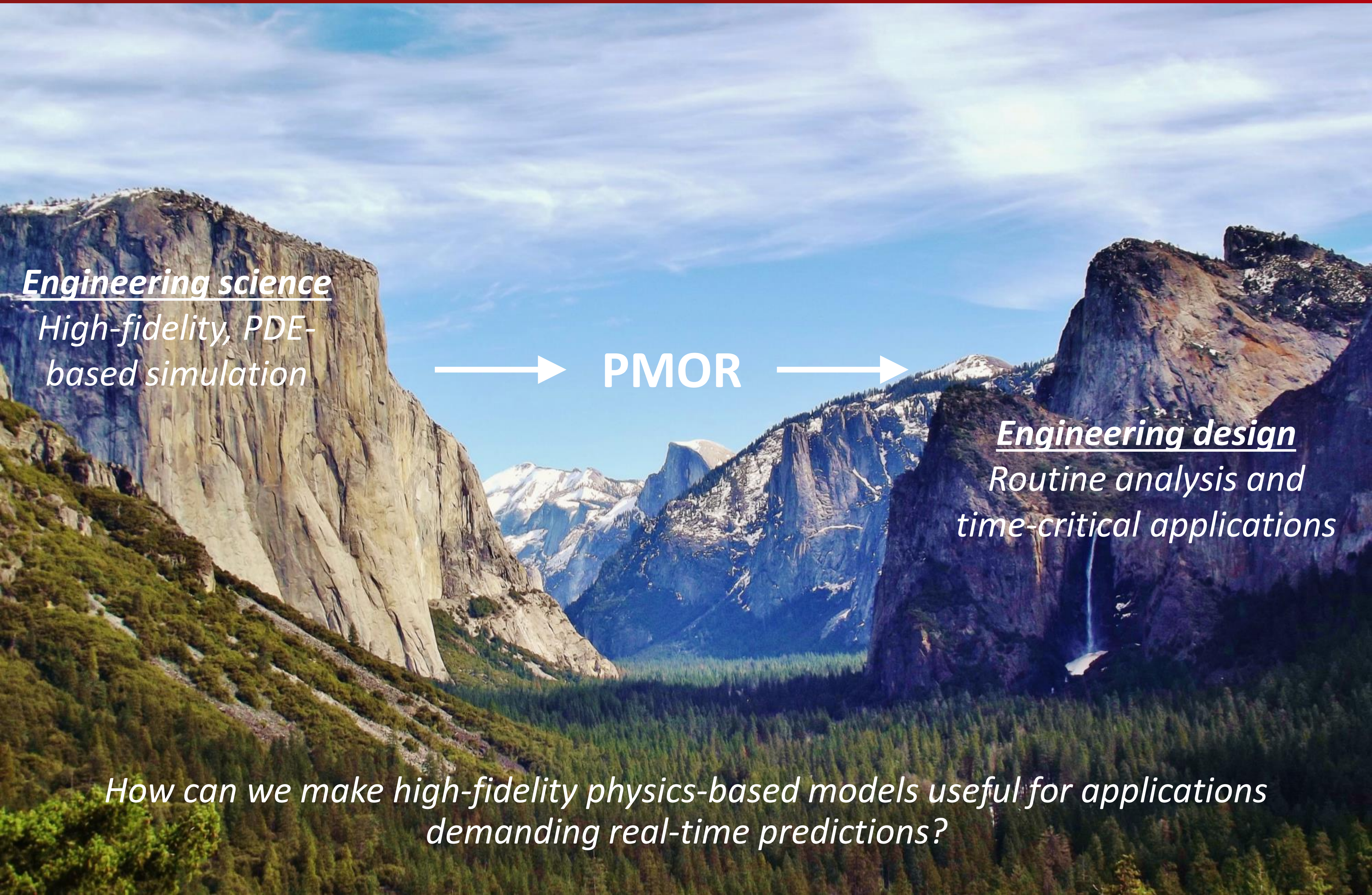
THE PERENIAL QUESTION OF COMPUTATIONAL EFFICIENCY

- Exascale computing and massive parallelism
  - Parachute simulation: 7 days on 2500 cores for 1 s of physical time

Pleiades, NASA Ames (#32 on TOP500)

- Processing time issues are exacerbated in the ***parametric*** setting

PROJECTION-BASED MODEL ORDER REDUCTION



PROJECTION-BASED MODEL ORDER REDUCTION

- High-dimensional, nonlinear, parametric computational models

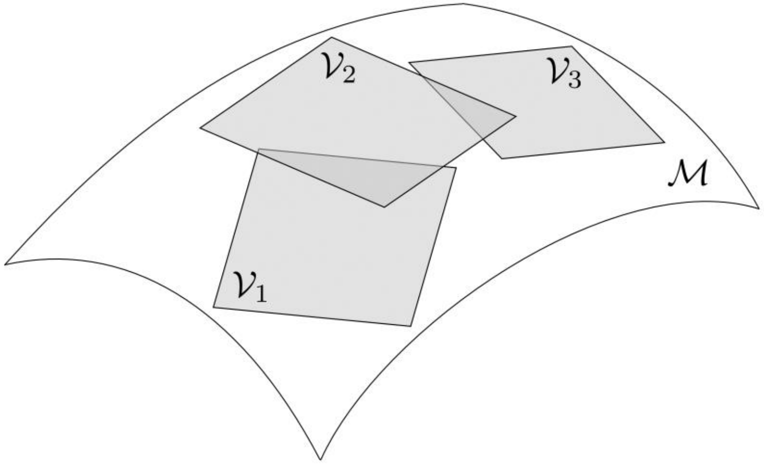
$$\boldsymbol{M}(\boldsymbol{\mu})\dot{\boldsymbol{u}} + \boldsymbol{f}(\boldsymbol{u};\boldsymbol{\mu}) = 0, \quad \boldsymbol{u}(t;\boldsymbol{\mu}) \in \mathbb{R}^N, \quad \boldsymbol{\mu} \in \mathcal{P} \subset \mathbb{R}^p$$

  - Prohibitively expensive to solve in many-query settings

- Solution approximation and dimensionality reduction
  - Trajectories of solutions to the ***high-dimensional*** model (HDM) often lie in ***low-dimensional*** subspaces
  - Data-driven approaches to discover ***reduced-order basis (ROB)*** for subspace

$$\boldsymbol{u}(t;\boldsymbol{\mu}) \approx \boldsymbol{V}\boldsymbol{y}(t;\boldsymbol{\mu})$$

$$\boldsymbol{V} \in \mathbb{R}^{N\times n}, \quad n \ll N$$



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Projection-based reduced-order model (PROM)

$$\underbrace{\boldsymbol{W}^T\boldsymbol{M}(\boldsymbol{\mu})\boldsymbol{V}}_{\boldsymbol{M}_n(\boldsymbol{\mu})}\,\dot{\boldsymbol{y}} + \underbrace{\boldsymbol{W}^T\boldsymbol{f}(\boldsymbol{V}\boldsymbol{y};\boldsymbol{\mu})}_{\boldsymbol{f}_n(\boldsymbol{y};\boldsymbol{\mu})} = 0$$

  - ***Divide and conquer:*** offline-online decomposition to enable efficient online simulations
  - Physics-based machine learning for acceleration of the HDM

OBSTACLES FOR PMOR

- ***Cost of training*** in offline stage: data collection costs from HDM and scalable algorithms for PROM construction

- ***Reducibility:*** finding accurate low-dimensional subspace approximations with n small enough for computational efficiency

- ***Stability:*** numerical stability of PROM operators does not necessarily follow from stability of the HDM

- ***Parametric dependence:*** implications for cost of training and reducibility

- ***Computational efficiency:*** low-dimensionality does not imply significant speedup factors for the nonlinear setting

PMOR FOR TURBULENT FLOW PROBLEMS

In the specific context of time-dependent, nonlinear, turbulent computational fluid dynamics (CFD) applications, focus on:

I. ***Reducibility:*** Convection-dominated and multiscale solution phenomena over large spatial and temporal ranges
  - Address concerns of modal truncation leading to ***numerical instability***

II. ***Computational efficiency:*** Treatment of nonpolynomial nonlinearities in HDM for PMOR of nonlinear CFD models to eliminate computational bottlenecks
  - Ensure associated training algorithms scale to reduce the ***cost of training***

PARAMETRIC PMOR (WASHABAUGH, 2016)

Boeing 777

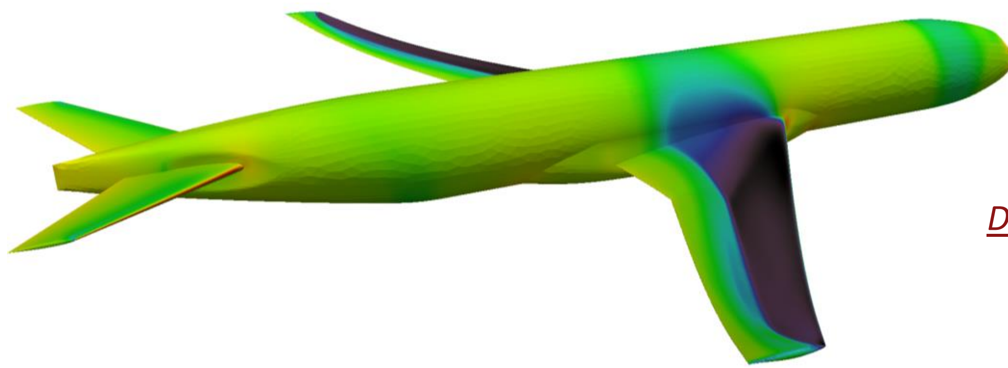
NASA Common Research Model (CRM)

PARAMETRIC PMOR (WASHABAUGH, 2016)

- Cruise conditions
  - M_∞ = 0.85, 2.32° angle of attack, Re = 5.0 × 10^6

- 3D steady-state RANS CFD model
  - Spalart-Allmaras turbulence model
  - Wall function
  - Unstructured mesh with 11.5M vertices

- Four-dimensional parameter space
  - Wingspan
  - Streamwise wingtip rake
  - Vertical wingtip rake
  - Outboard twist (washout)



<u>Drag</u> *Baseline: 141.01 kN*
What-if: 141.76 kN

- "What-if" scenarios to pave the way for automated optimization

TOTAL COMPUTATIONAL OVERHEAD

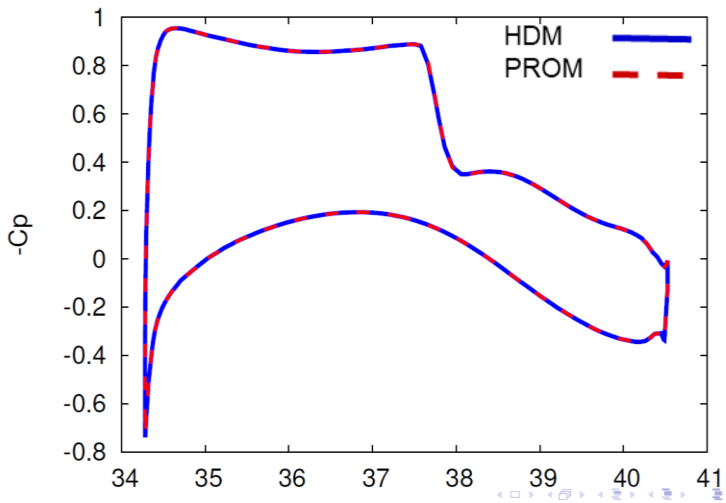
- Training on Excalibur (Cray XC40, U.S. ARL)
  - 1,024 cores assigned to each of 24 sampled configurations
  - 2 hrs wall-clock time per sampled parameter point → embarrassingly parallel
  - 14.6 min wall-clock time for constructing global ROB and PROM on 1,024 cores

Wall-clock time investment: 2 hrs on 24,576 cores
+ 14.6 min on 1,024 cores

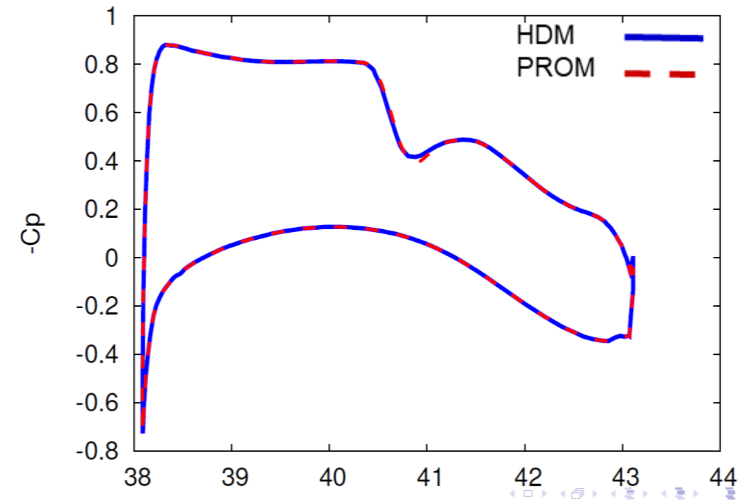
ONLINE PERFORMANCE

- Global PROM accuracy for parameter query at center of design space

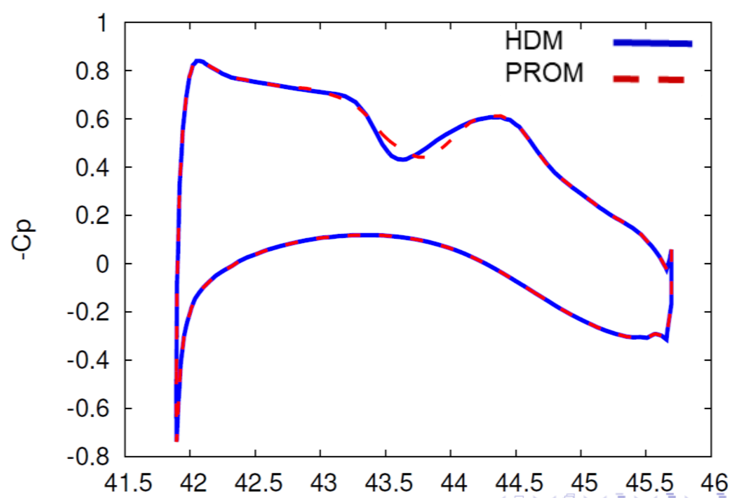
15 m



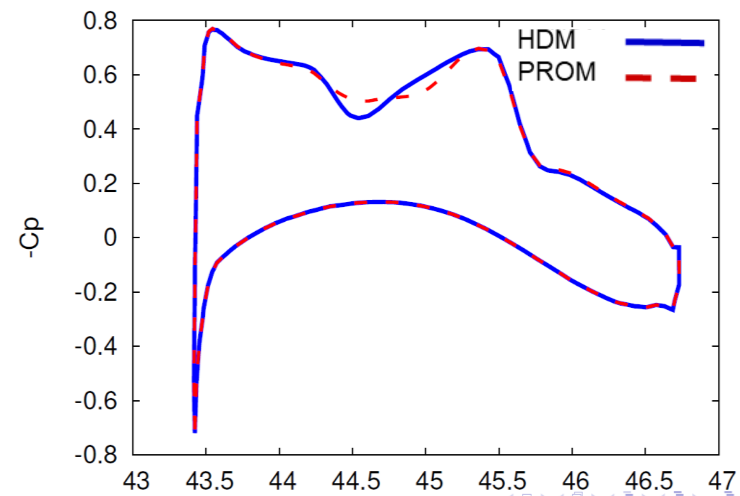
20 m



25 m

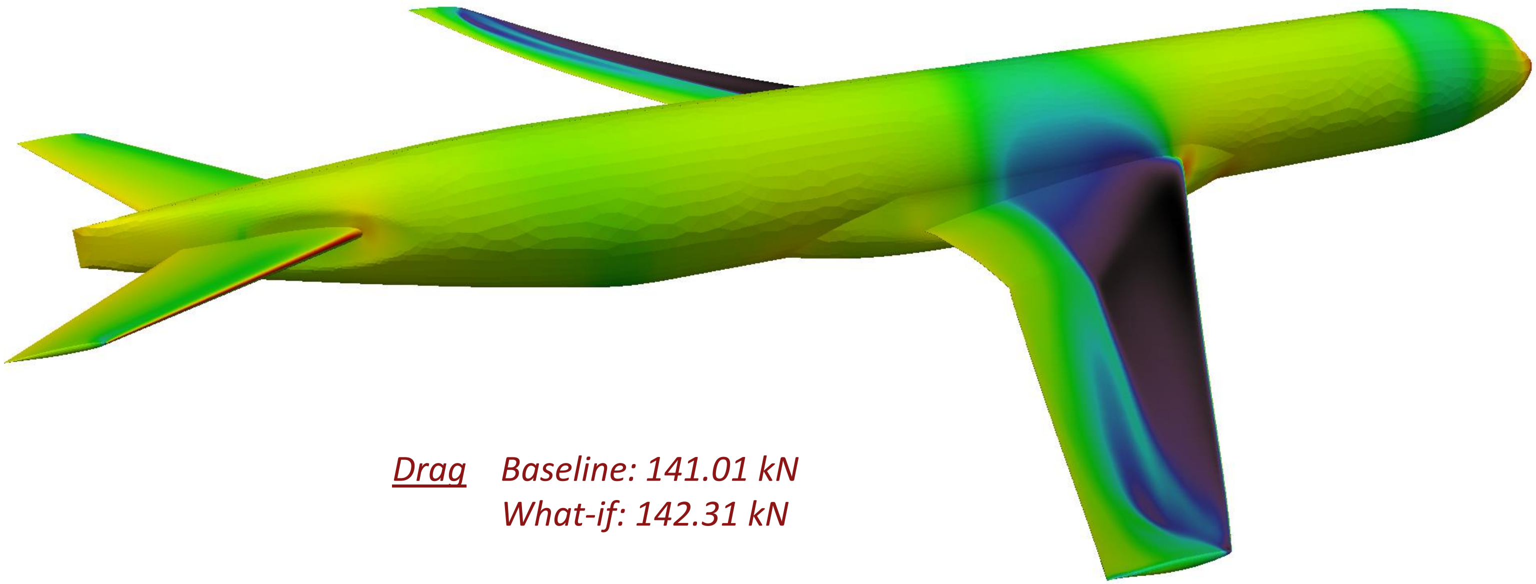


27 m



ONLINE PERFORMANCE

- Parameter query at center of design space
  - Near real-time prediction: PROM solution in ***2.8 min*** on a laptop

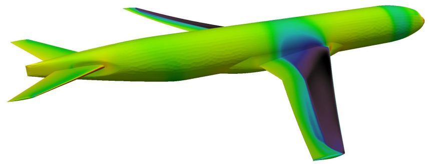


<u>Drag</u> *Baseline: 141.01 kN*
What-if: 142.31 kN

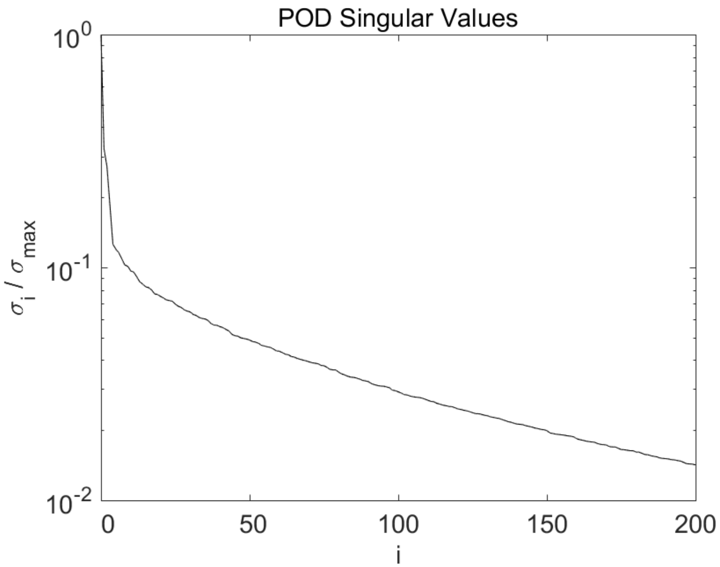
I. On Numerical Stability for Convection-Dominated Problems

NONLINEAR HYPERBOLIC PROBLEMS

- What about ***scale-resolving*** turbulent flow models?
  - Large eddy simulation (LES)
  - Direct numerical simulation (DNS)



- Convection-dominated problems $\rightarrow$ ***not exactly low-rank***
  - Slow convergence of snapshot matrix singular values characteristic of slowly decaying Kolmogorov n-width of HDM solution manifold



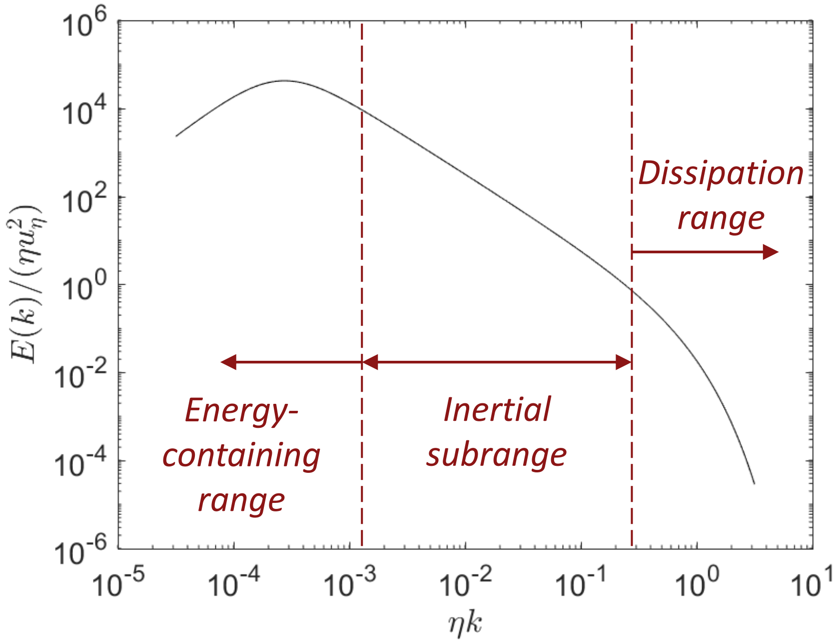
Modal truncation

$$\boldsymbol{u} \approx \sum_{i=1}^{n} \boldsymbol{V}_i \boldsymbol{y}_i \quad \rightarrow$$

Trade-off between large n required for accuracy, or small n for speed

TURBULENCE

- Turbulent energy cascade (Kolmogorov, 1941)

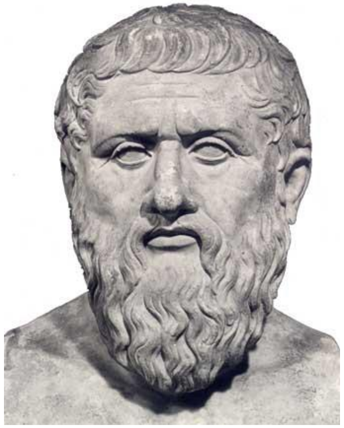


- ***Recurrent claim for turbulent PROMs:*** modal truncation eliminates viscous dissipation mechanisms and therefore artificially destabilizes the computation
  - Only supported by numerical evidence using in ALL cases PROMs based on ***Galerkin projection*** (left ROB $\boldsymbol{W} = \boldsymbol{V}$)
  - Here, the case is made that Galerkin projection is to blame for instability, rather than physical cascade argument

PMOR AS A SEMI-DISCRETIZATION METHOD

- “We do not learn, and that what we call learning is only a process of recollection”

- PMOR is a ***Ritz method*** (1909) where the global basis functions are constructed *a posteriori* after some knowledge about the parametrized system is developed, instead of being selected *a priori* $\rightarrow$ ***learning vs. postulation***



Plato

SEMI-DISCRETIZATION FOR CONVECTION-DOMINATED FLOW PROBLEMS

- Consider the linear advection-diffusion equation

$$\begin{cases} \dot{u} + \nabla \cdot (\boldsymbol{a} u - \nu \nabla u) = f & \text{in } \Omega \times [0, T] \\ u = 0 & \text{on } \Gamma_g \times [0, T] \\ u(\boldsymbol{x}, 0) = u_0 & \text{in } \Omega \end{cases}$$

- Error estimate for Galerkin finite element method with standard polynomial approximations of order k

$$\|\nabla(u - u_h)\|_{L^2(\Omega)} = O((1 + Pe_h)h^k)$$

Instability

- Streamline-upwind ***Petrov-Galerkin*** (SUPG) method (1982)
  - Use different test/trial function spaces to achieve numerical stability

PETROV-GALERKIN PROJECTION

- Right (test) ROB $\boldsymbol{V}$ is constructed for optimal accuracy, left (trial) ROB $\boldsymbol{W}$ enforces uniqueness of the solution ***as well as any desired additional constraints***

- In the linear case: Petrov-Galerkin projection to ensure PROM satisfies Lyapunov stability criterion for LTI systems (Amsallem and Farhat, 2012)

- In the nonlinear case: ***time-discrete residual minimization***

$$\boldsymbol{W}^T \hat{\boldsymbol{r}}(\boldsymbol{V}\boldsymbol{y}^{m+1}, t^{m+1}; \boldsymbol{\mu}) = 0 \quad \Leftrightarrow \quad \boldsymbol{y}^{m+1} = \underset{\boldsymbol{x}\in\mathbb{R}^n}{\arg\min} \|\hat{\boldsymbol{r}}(\boldsymbol{V}\boldsymbol{x}, t^{m+1}; \boldsymbol{\mu})\|_{\boldsymbol{\Theta}}$$

1. $\boldsymbol{W} = \boldsymbol{V} \quad \rightarrow$ ***Galerkin*** projection: $\boldsymbol{\Theta} = (\boldsymbol{J}^{m+1})^{-1}$, only if inverse of Jacobian is symmetric positive definite (SPD)
2. $\boldsymbol{W} = \boldsymbol{\Theta}\boldsymbol{J}^{m+1}\boldsymbol{V} \rightarrow$ ***Petrov-Galerkin*** projection: equivalence for *any* SPD $\boldsymbol{\Theta}$

- $\boldsymbol{\Theta} = \boldsymbol{I} \rightarrow$ ***Least-squares Petrov-Galerkin (LSPG):*** Gauss-Newton method for nonlinear least-squares

SUPPORTING NUMERICAL EXAMPLES

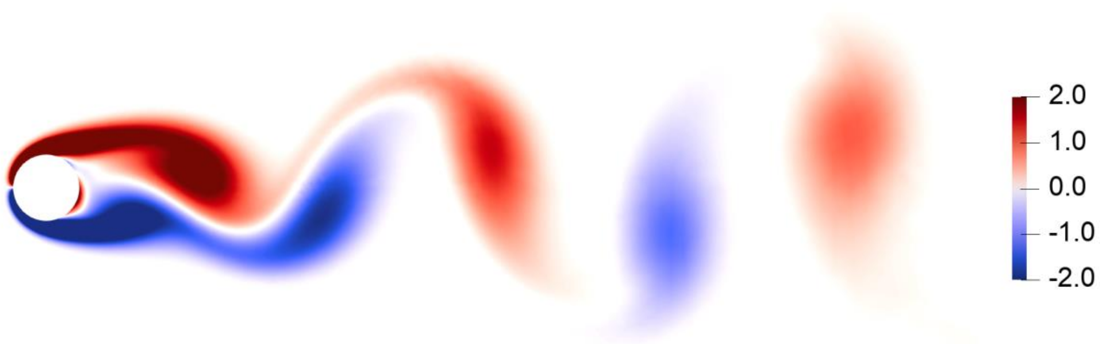
- Several numerical examples demonstrate falseness of the truncation-based instability claim
  - Example #1: Galerkin PROMs unstable even in the absence of turbulence for convection-dominated problems
  - Example #2: Galerkin PROMs stable even with severe modal truncation when non-convection-dominated

- Petrov-Galerkin PROMs using the LSPG projection will be shown to be numerically stable (and accurate) in all cases

2D LAMINAR FLOW OVER A CIRCULAR CYLINDER

- At Re = 100 and M_∞ = 0.2, flow exhibits periodic vortex shedding after transient startup
  - Time integration in nondimensional time interval [0, 200], where flow becomes periodic at t = 100

- HDM characterization
  - Compressible Navier-Stokes equations semi-discretized using a second-order mixed FV/FE scheme
  - Implicit time discretization using second-order DIRK scheme
  - Resulting dimension ***N* = 490,700**



Solution vorticity snapshot

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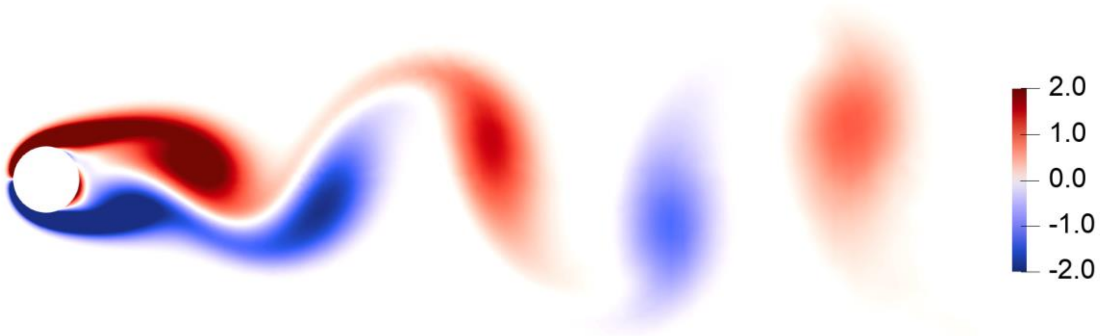
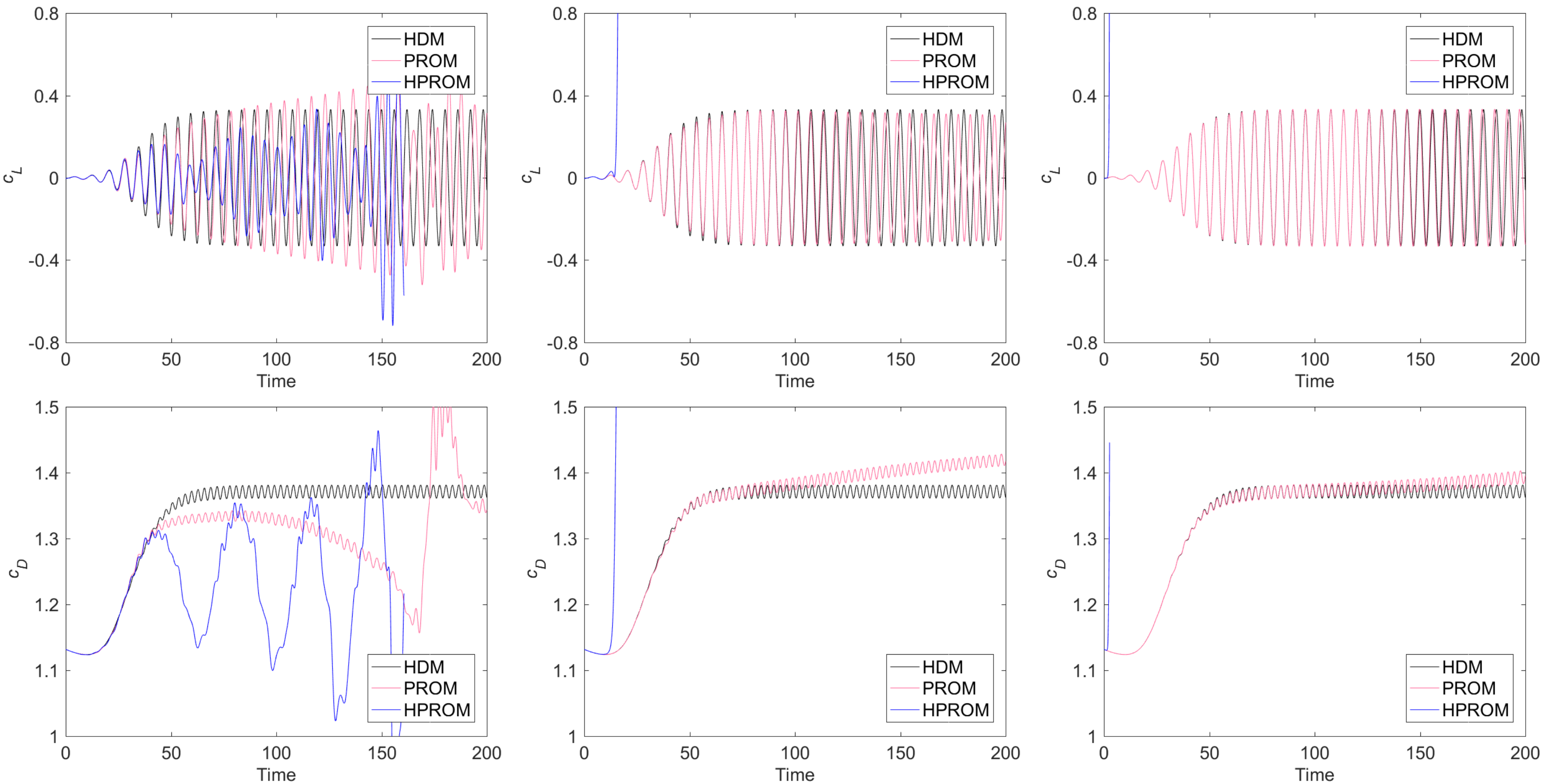
- Galerkin and Petrov-Galerkin PROMs
  - Least-squares Petrov-Galerkin (LSPG) projection
  - 751 collected solution snapshots from $t \in [0, 150]$
  - 3 ROB dimensions for constructing Galerkin and LSPG PROMS: ***n* = 20, 35,** and ***55***, corresponding to 99.9%, 99.99%, and 99.999% of snapshot matrix singular value energy



Solution vorticity snapshot

2D LAMINAR FLOW OVER A CIRCULAR CYLINDER

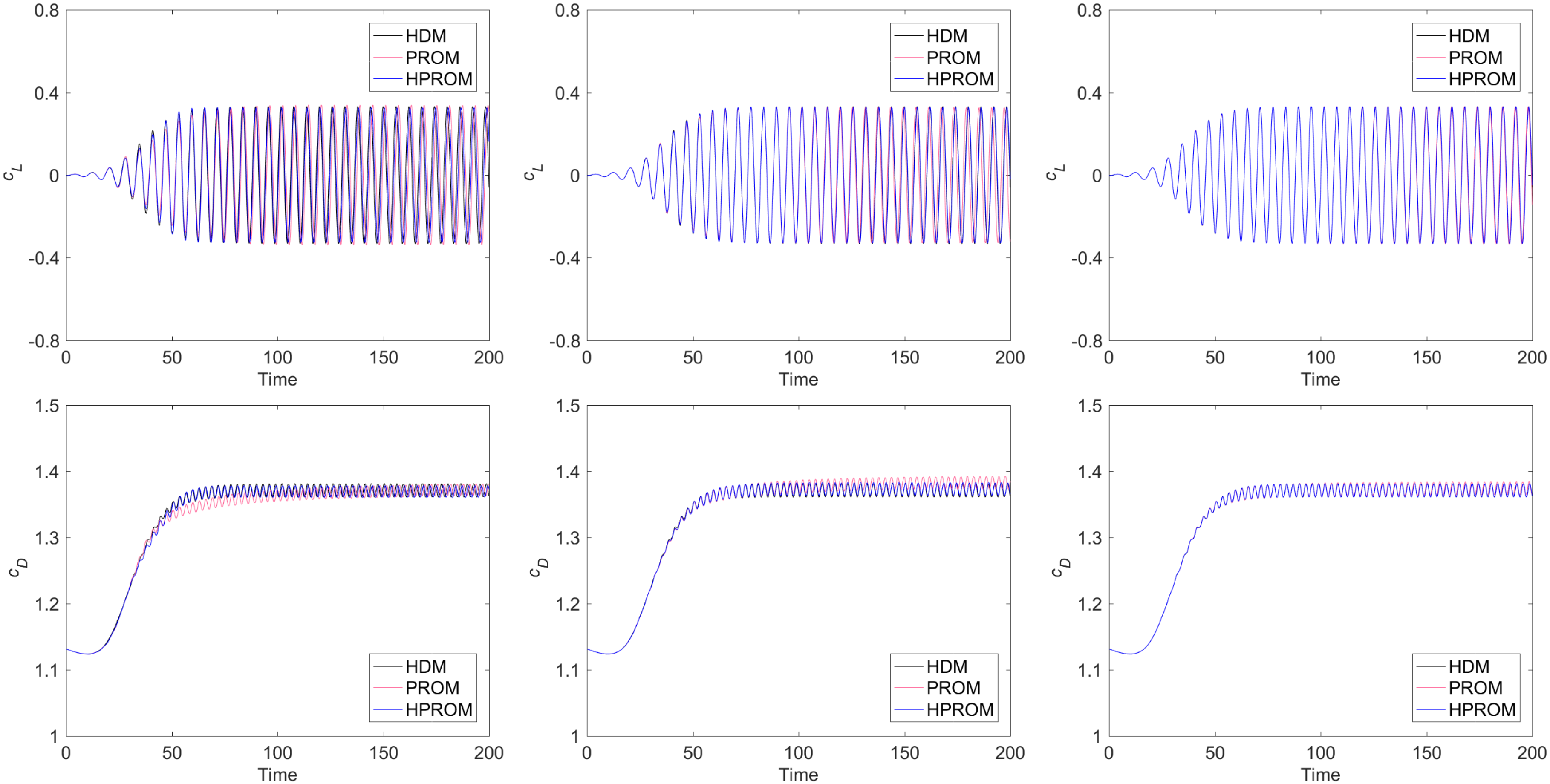
- Comparison of time histories of lift and drag coefficients for Galerkin PROMs



Galerkin, n = 20 | Galerkin, n = 35 | Galerkin, n = 55

2D LAMINAR FLOW OVER A CIRCULAR CYLINDER

- Comparison of time histories of lift and drag coefficients for Petrov-Galerkin PROMs

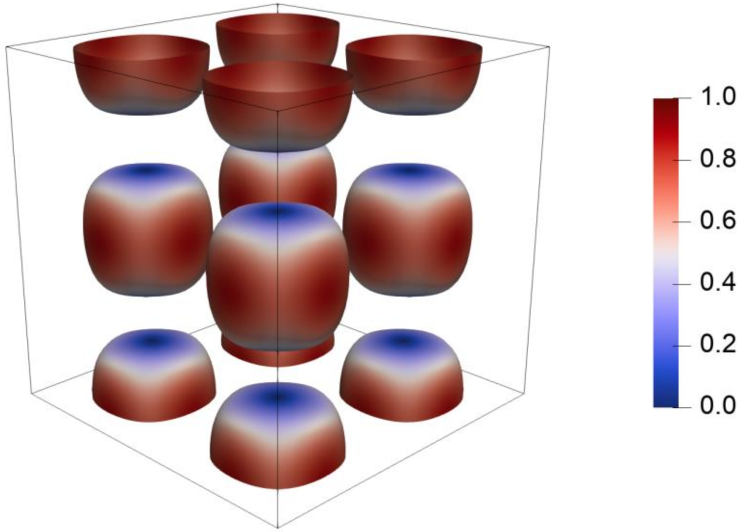


LSPG, n = 20

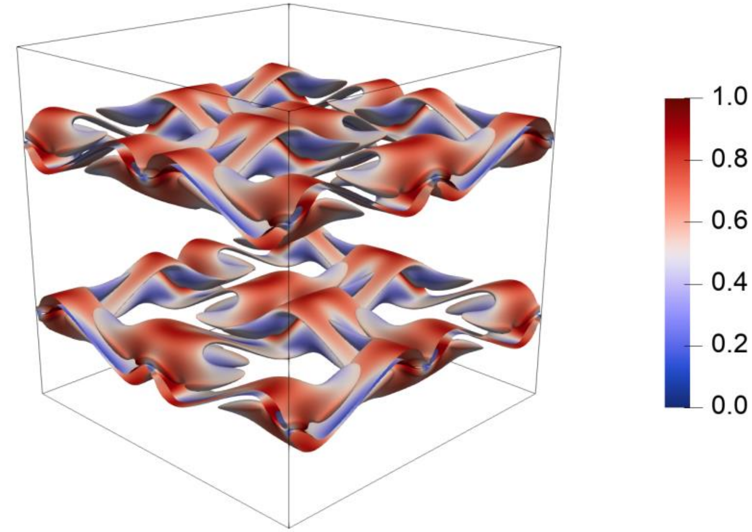
LSPG, n = 35

LSPG, n = 55

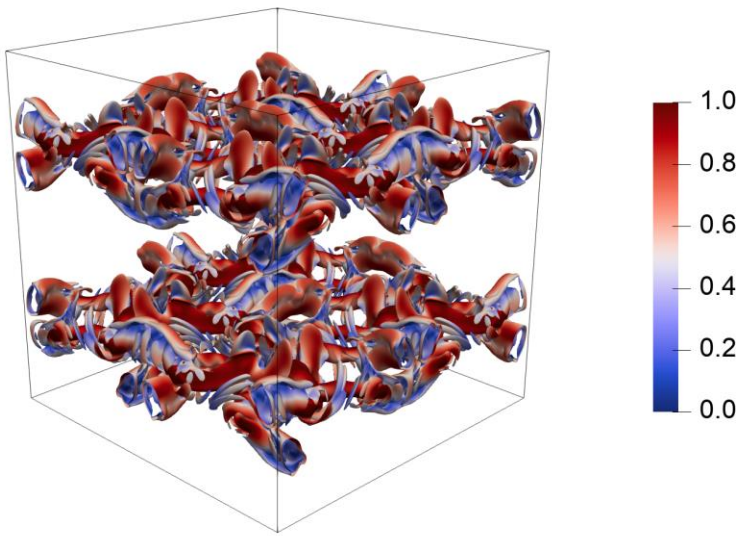
TAYLOR-GREEN VORTEX PROBLEM



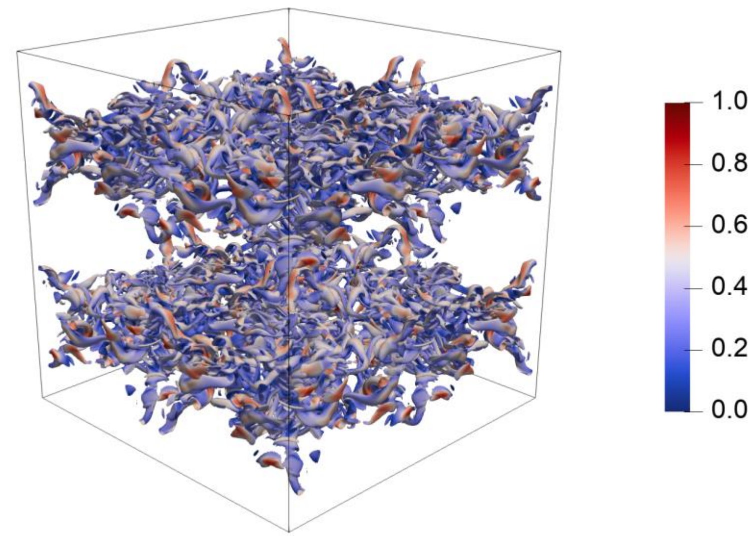
$t = 0$



$t = 4$



$t = 8$



$t = 12$

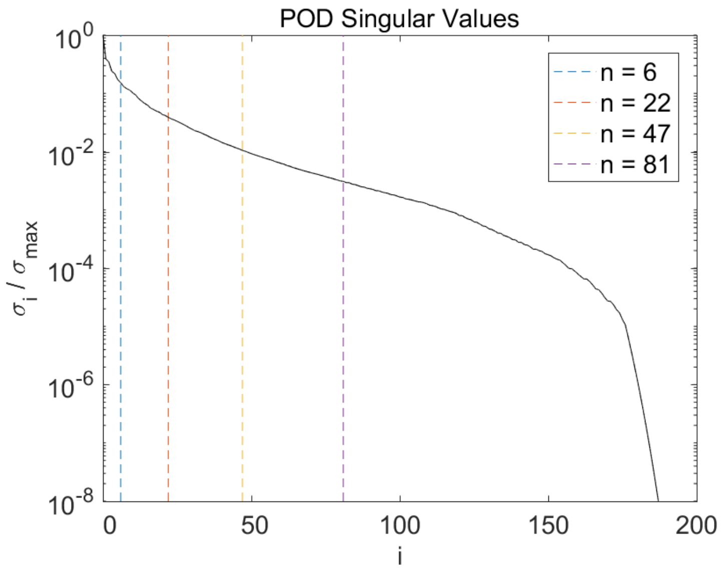
TAYLOR-GREEN VORTEX PROBLEM

- Homogeneous, isotropic turbulence in a triply-periodic box of side-length 2π at Re = 1,600
  - Canonical flow often used as benchmark problem for evaluating numerical schemes and their ability to simulate turbulence
  - In nondimensional time interval [0, 20], vortices decay into turbulence
  - ***Multiscale*** flow transition used to study effects of ROB truncation on PROM accuracy and stability

- HDM construction
  - Pseudospectral Fourier-Galerkin method for DNS of the incompressible Navier-Stokes equations
  - 512 grid points per spatial direction yields $\boldsymbol{N}$ ***= 402,653,183***
  - Time integration using explicit RK4 for snapshot collection with nondimensional time step Δt = 0.001

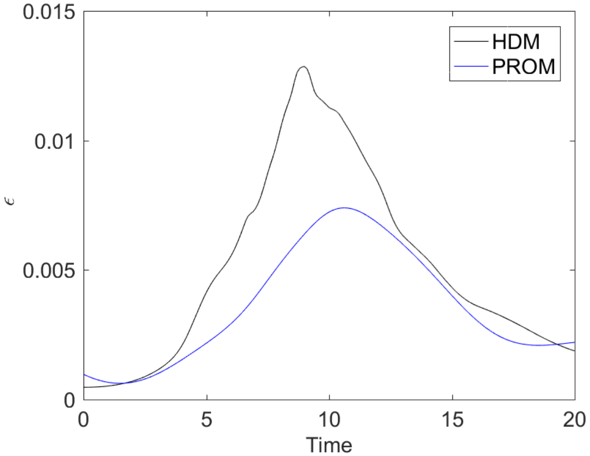
TAYLOR-GREEN VORTEX PROBLEM

- Galerkin and Petrov-Galerkin PROM construction
  - 201 solution snapshots collected at Δs = 0.1 from HDM for ROB construction via POD
  - 4 Galerkin and LSPG PROMs of dimension ***n* = 6, 22, 47,** and ***81*** corresponding to energy thresholds from 90% to 99.99%
  - All PROMs employ implicit four-point BDF scheme for time discretization

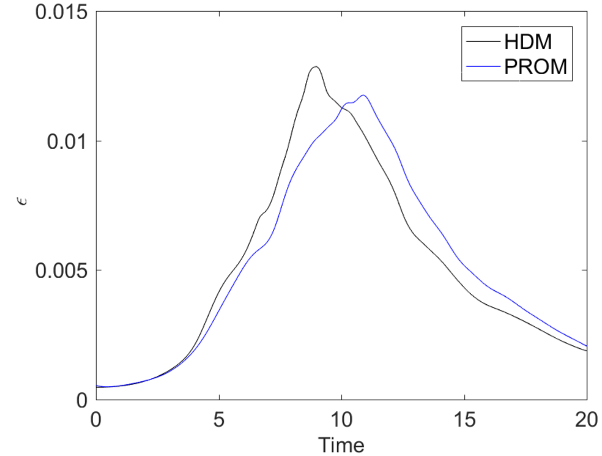


TAYLOR-GREEN VORTEX PROBLEM

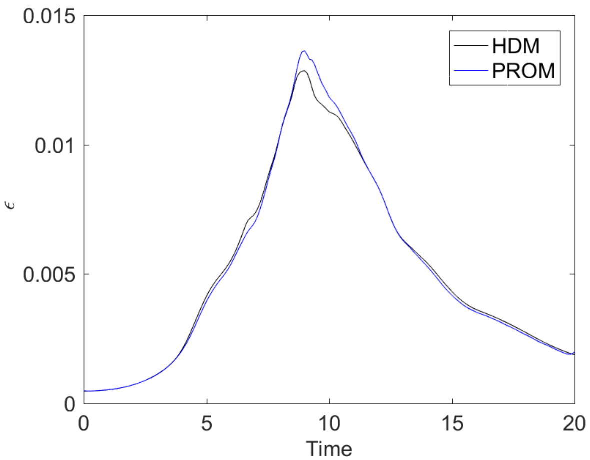
- Comparison of time histories of the enstrophy-based dissipation rate computed using the HDM and Galerkin PROMs



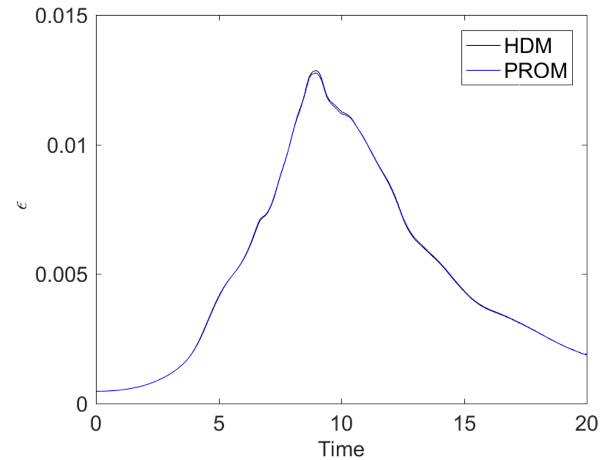
Galerkin, n = 6



Galerkin, n = 22



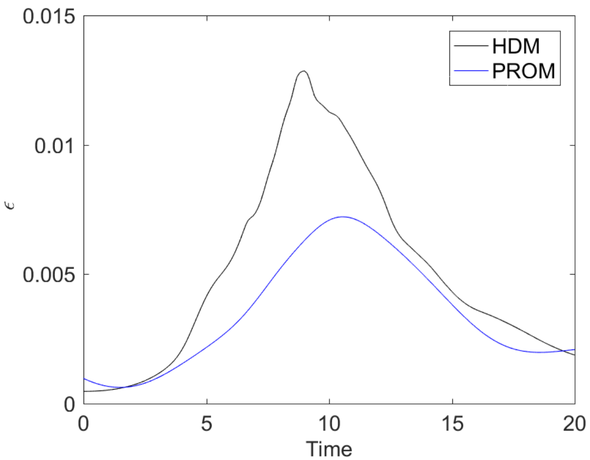
Galerkin, n = 47



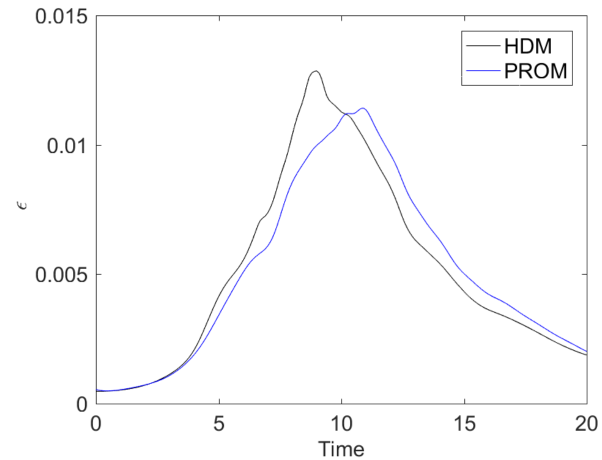
Galerkin, n = 81

TAYLOR-GREEN VORTEX PROBLEM

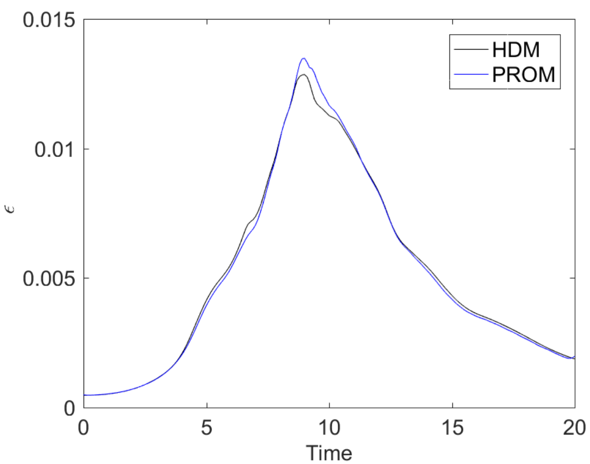
- Comparison of time histories of the enstrophy-based dissipation rate computed using the HDM and Petrov-Galerkin PROMs



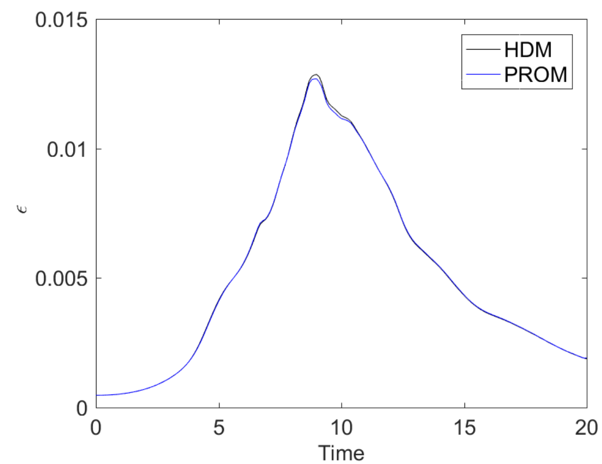
LSPG, n = 6



LSPG, n = 22



LSPG, n = 47



LSPG, n = 81

TAYLOR-GREEN VORTEX PROBLEM

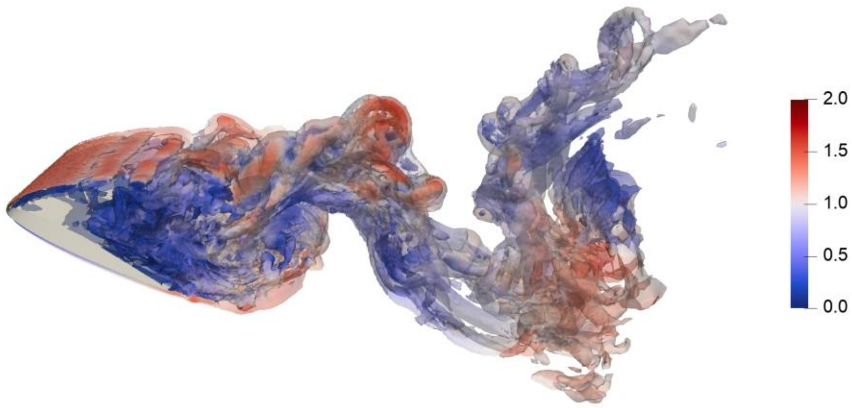
- Some pertinent observations
  - Both Galerkin and LSPG PROMs deliver similar performance and are numerically stable for all values of n
  - Very high degree of accuracy achieved for $\boldsymbol{n = 81}$**,** versus HDM dimension $\boldsymbol{N = 402{,}653{,}183}$**,** even for complex multiscale physics

- LSPG PROM speedup factors vs. HDM

Model	n	*Wall-clock time (# cores)*	*Wall-clock time speedup factor*	*CPU time speedup factor*
HDM		34.9 hrs (128)	-	-
PROM	6	6.0 s (1)	**21,100**	**2,700,000**
	22	14.8 s (1)	**8,480**	**1,090,000**
	47	1.2 min (1)	**1,820**	**233,000**
	81	8.1 min (1)	**258**	**33,100**

LES OF FLOW PAST AN EXTRUDED AIRFOIL

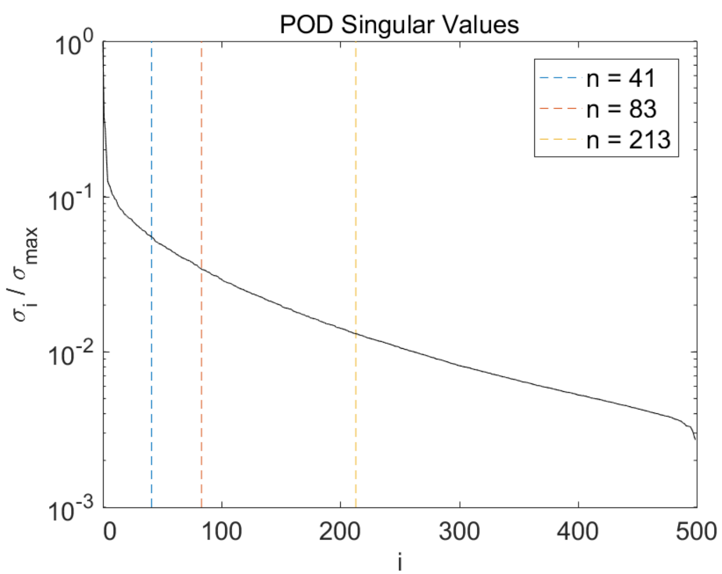
- NACA 0012, Re = 10,000, M_∞ = 0.2, 30° angle of attack
  - Compute vortex shedding solution for 30 nondimensional time units
- Spatial and time discretization
  - Vreman (2004) subgrid-scale turbulence model
  - ***Fifth-order*** low-diffusion finite volume scheme for convective terms, ***second-order*** Galerkin finite element scheme for diffusive terms
  - Time discretization using ***third-order*** DIRK scheme
- Computational domain
  - One-chord length extrusion in spanwise direction, periodic BC on spanwise faces
  - Unstructured mesh with 2.1M vertices, 11.9M tetrahedra
  - HDM dimension ***N = 10,397,730***



Contours of vorticity magnitude colored by Mach number

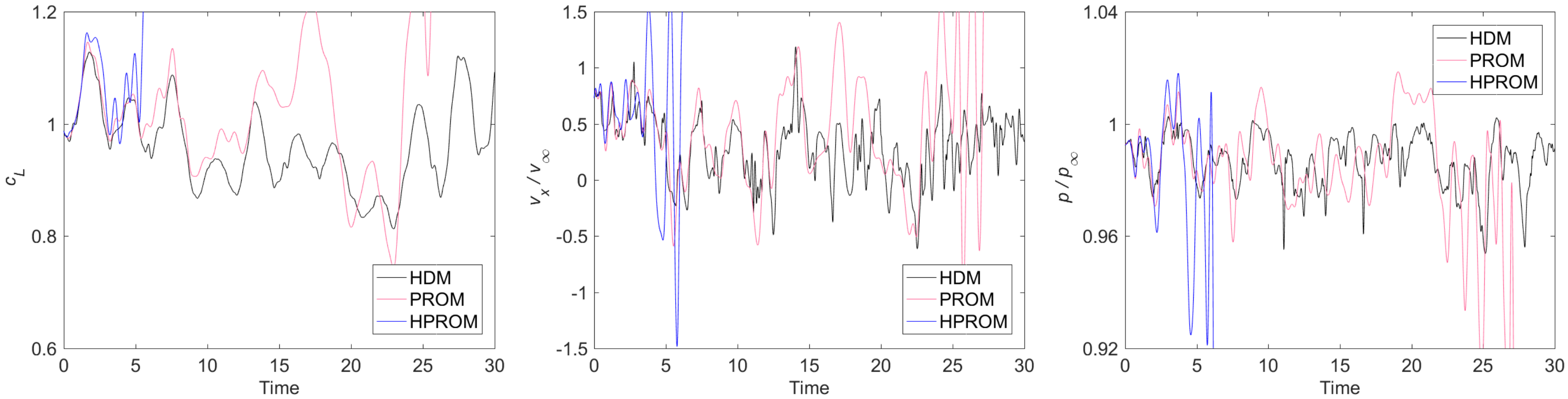
LES OF FLOW PAST AN EXTRUDED AIRFOIL

- PROM construction
  - HDM solution snapshots collected at $\Delta s = 0.06 \rightarrow$ 501 snapshots
  - Right ROB of dimension $\boldsymbol{n = 83}$ computed via POD, corresponding to singular value energy threshold of 95%
  - Galerkin and LSPG PROMs



LES OF FLOW PAST AN EXTRUDED AIRFOIL

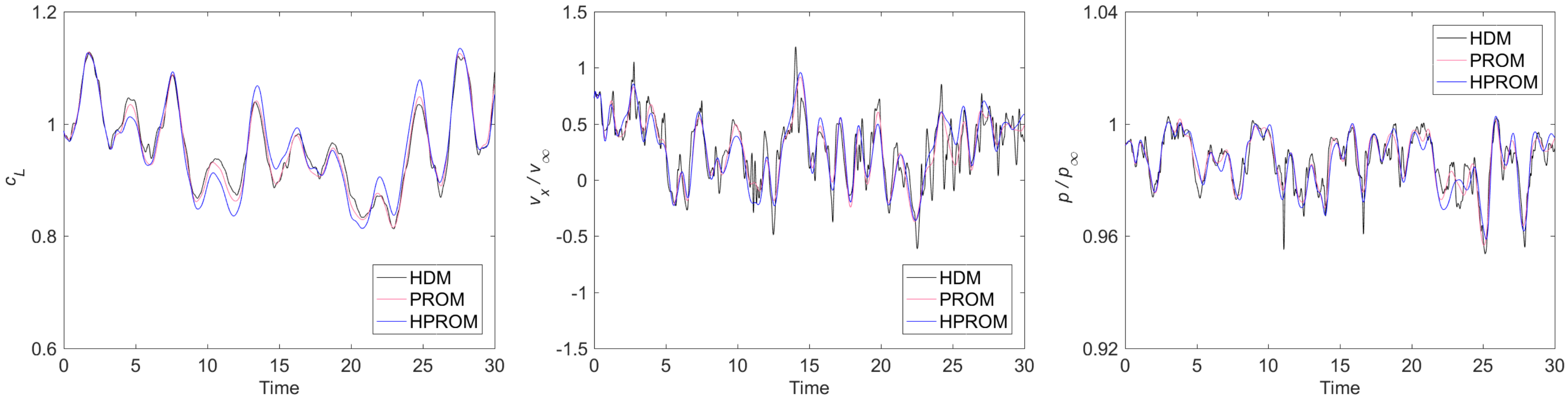
- Comparison of lift coefficient and streamwise velocity and pressure computed at a probe using the HDM and Galerkin PROM
  - Probe is located 1.5 chord lengths downstream from airfoil TE



- Galerkin PROMs are numerically unstable for all considered ROB dimensions

LES OF FLOW PAST AN EXTRUDED AIRFOIL

- Comparison of lift coefficient and streamwise velocity and pressure computed at a probe using the HDM and Petrov-Galerkin PROM
  - Probe is located 1.5 chord lengths downstream from airfoil TE



- LSPG PROMs are stable, and maintain stability and accuracy when hyperreduction is introduced

SUMMARY AND CONCLUSIONS, PART I

- ***Proving vs. disproving:*** LSPG projection is/can be stable for nonlinear PMOR of scale-resolving turbulent flow models
  - Galerkin projection can also produce stable and accurate PROMs, but only where appropriate: not well-suited for convection-dominated problems

- ***Physics vs. numerics:*** explaining numerical behavior using only physics-based arguments is not necessarily justifiable and can lead to the wrong conclusions

II. Computational Bottlenecks and Hyperreduction

PROM CONSTRUCTION

- Recall the semi-discrete nonlinear HDM

$$\boldsymbol{M}(\boldsymbol{\mu})\dot{\boldsymbol{u}} + \boldsymbol{f}(\boldsymbol{u};\boldsymbol{\mu}) = 0, \qquad \boldsymbol{u}(t;\boldsymbol{\mu}) \in \mathbb{R}^N$$

and linear (global) subspace approximation

$$\boldsymbol{u}(t;\boldsymbol{\mu}) \approx \boldsymbol{V}\boldsymbol{y}(t;\boldsymbol{\mu}), \qquad \boldsymbol{V} \in \mathbb{R}^{N\times n}, \qquad n \ll N$$

PROM CONSTRUCTION

- Constructing a ***Petrov-Galerkin PROM*** of dimension n

$$\boldsymbol{r}(\boldsymbol{V}\boldsymbol{y}, \boldsymbol{V}\dot{\boldsymbol{y}}; \boldsymbol{\mu}) = \boldsymbol{M}(\boldsymbol{\mu})\boldsymbol{V}\dot{\boldsymbol{y}} + \boldsymbol{f}(\boldsymbol{V}\boldsymbol{y}; \boldsymbol{\mu}) \neq 0 \qquad \leftarrow \textit{Dimension } N$$

$$\downarrow$$

$$\boldsymbol{W}^T\boldsymbol{r} = 0$$

$$\downarrow$$

PROM:

$$\underbrace{\boldsymbol{W}^T\boldsymbol{M}(\boldsymbol{\mu})\boldsymbol{V}}_{\boldsymbol{M}_n(\boldsymbol{\mu})}\dot{\boldsymbol{y}} + \underbrace{\boldsymbol{W}^T\boldsymbol{f}(\boldsymbol{V}\boldsymbol{y}; \boldsymbol{\mu})}_{\boldsymbol{f}_n(\boldsymbol{y};\boldsymbol{\mu})} = 0 \qquad \leftarrow \textit{Dimension } n \ll N$$

  - Even though PROM is low-dimensional, solution can be more expensive than the HDM!

- Polynomial nonlinearities admit precomputable decomposition

$$\boldsymbol{W}^T\boldsymbol{f}(\boldsymbol{V}\boldsymbol{y}; \boldsymbol{\mu}) = \underbrace{\boldsymbol{W}^T\boldsymbol{G}(\boldsymbol{V})}_{\textit{precomputable}}\boldsymbol{h}(\boldsymbol{y}; \boldsymbol{\mu})$$

ISSUES WITH NONLINEARITY

- For the general nonlinear case, solution of the PROM is ***still expensive***
  - Must reconstruct high-dimensional state, compute high-dimensional nonlinear function, then project onto low-dimensional space

$$(\boldsymbol{y}, \dot{\boldsymbol{y}}) \rightarrow (\boldsymbol{V}\boldsymbol{y}, \boldsymbol{V}\dot{\boldsymbol{y}}) \rightarrow \boldsymbol{r}(\boldsymbol{V}\boldsymbol{y}, \boldsymbol{V}\dot{\boldsymbol{y}}; \boldsymbol{\mu}) \rightarrow \boldsymbol{W}^T\boldsymbol{r}(\boldsymbol{V}\boldsymbol{y}, \boldsymbol{V}\dot{\boldsymbol{y}}; \boldsymbol{\mu})$$

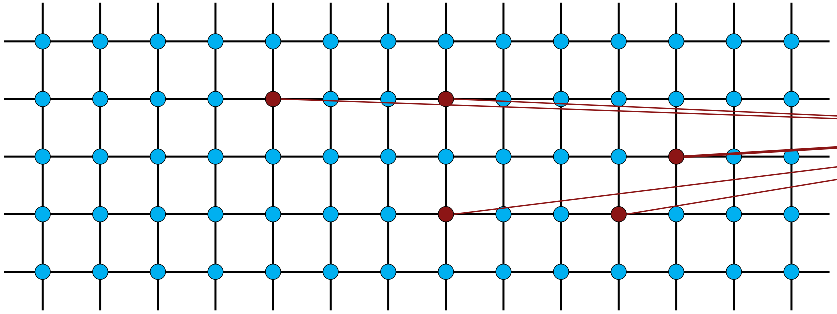
  - $O(Nn)$ at every linearization, every time step, every new parameter query

- ***Hyperreduction:*** a second-layer approximation introduced to accelerate evaluation of nonlinear models
  - Remove complexity scaling with N
  - Raison d’être goes beyond just state nonlinearities: linear stochastic PROMs, nonaffine parameter dependence

HYPERREDUCTION OF NONLINEAR PROMS

- ***Approximate-then-project*** hyperreduction methods
  - Empirical interpolation approaches based on the gappy proper orthogonal decomposition (POD) method (1995)
  - Common 3-step idea:

1. Compute function at only a few spatial locations:



$$\boldsymbol{f}^{\mathcal{I}}(\boldsymbol{V}\boldsymbol{y};\boldsymbol{\mu})$$

2. Interpolate using empirical basis functions: $\boldsymbol{f}(\boldsymbol{V}\boldsymbol{y};\boldsymbol{\mu}) \approx \boldsymbol{V}_{\boldsymbol{f}}\boldsymbol{g}(\boldsymbol{f}^{\mathcal{I}})$
3. Compute the projected approximation: $\boldsymbol{f}_r = \boldsymbol{W}^T\boldsymbol{f} \approx \boldsymbol{W}^T\boldsymbol{V}_{\boldsymbol{f}}\boldsymbol{g}(\boldsymbol{f}^{\mathcal{I}})$

  - State-of-the-art for many PMOR frameworks, including CFD
  - Standard implementations rely on suboptimal ***greedy mesh sampling algorithms*** and only consider accuracy of high-dimensional interpolation

HYPERREDUCTION OF NONLINEAR PROMS

- ***Project-then-approximate*** hyperreduction methods
  - Approximate the projected reduced-order quantities directly
  - Interpretation as empirical generalized quadrature rules

- Example: ***energy-conserving sampling and weighting (ECSW)*** (2014)
  - Developed for second-order finite element models in computational structural dynamics

$$\int_{\Omega} f(u) v \, d\boldsymbol{x} = \sum_{e \in \mathcal{E}} \int_{\Omega_e} f(u) v \, d\boldsymbol{x} \approx \sum_{e \in \widetilde{\mathcal{E}} \subset \mathcal{E}} \xi_e \int_{\Omega_e} f(u) v \, d\boldsymbol{x}, \qquad |\widetilde{\mathcal{E}}| \ll |\mathcal{E}|$$

  - Unique structure preserving and stability properties

ECSW FOR TURBULENT FLOW MODELS

- Can we generalize the ECSW method to accelerate nonlinear PROMs for CFD applications?
  - First-order systems of conservation laws
  - Arbitrary underlying semi-discretizations
  - Training algorithms for *very* high-dimensional problems
  - Is $|\tilde{\mathcal{E}}| \ll |\mathcal{E}|$ possible for complex, turbulent flow applications?

ECSW FOR TURBULENT FLOW MODELS

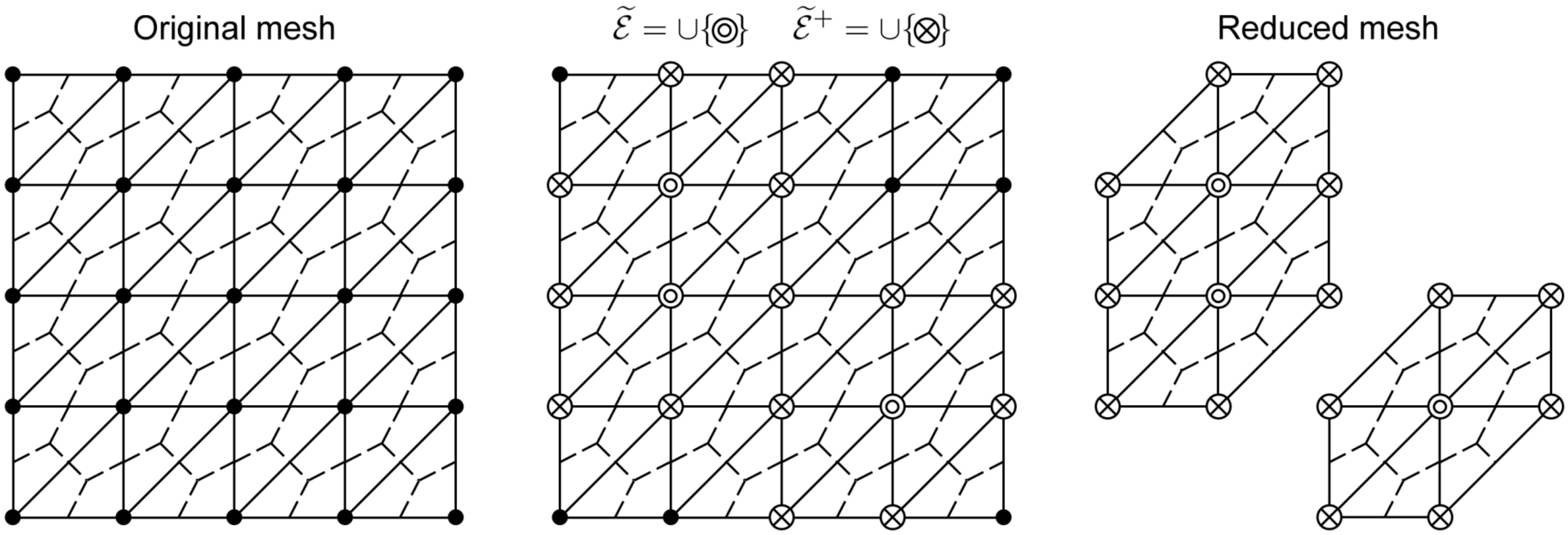
- ECSW approximation for general Petrov-Galerkin PROMs

$$\boldsymbol{W}^T\boldsymbol{r}(\boldsymbol{V}\boldsymbol{y},\boldsymbol{V}\dot{\boldsymbol{y}};\boldsymbol{\mu}) = \sum_{e\in\mathcal{E}} \boldsymbol{W}^T\boldsymbol{L}_e^T\boldsymbol{r}_e(\boldsymbol{L}_{e^+}\boldsymbol{V}\boldsymbol{y},\boldsymbol{L}_{e^+}\boldsymbol{V}\dot{\boldsymbol{y}};\boldsymbol{\mu})$$

$$\approx \sum_{e\in\widetilde{\mathcal{E}}\subset\mathcal{E}} \xi_e\boldsymbol{W}^T\boldsymbol{L}_e^T\boldsymbol{r}_e(\boldsymbol{L}_{e^+}\boldsymbol{V}\boldsymbol{y},\boldsymbol{L}_{e^+}\boldsymbol{V}\dot{\boldsymbol{y}};\boldsymbol{\mu})$$

  - $\boldsymbol{L}_e$ is a boolean localization matrix to the DOFs corresponding to mesh entity e
  - Computations take place on a ***reduced mesh*** defined by $\tilde{\mathcal{E}}$, which can represent a subset of the high-dimensional mesh elements, dual-cells, collocation points, or any required geometric entity as per the HDM semi-discretization

ECSW FOR TURBULENT FLOW MODELS



OPTIMAL SAMPLE WEIGHT COMPUTATION

- How to compute the sampled entities $\tilde{\mathcal{E}}$ and the associated weights ξ_e?

- Consider a set of training snapshots $\{\boldsymbol{u}^{(i)}, \dot{\boldsymbol{u}}^{(i)}\}_{i=1}^{N_t}, \ \boldsymbol{u}^{(i)} = \boldsymbol{u}(t^p; \boldsymbol{\mu}^q)$
  - Assemble training data in matrix form representing the $\boldsymbol{W}^T\boldsymbol{r}$ operation over all N_t training samples

$$\begin{bmatrix} \boldsymbol{c}_{11} & \cdots & \boldsymbol{c}_{1|\mathcal{E}|} \\ \vdots & \ddots & \vdots \\ \boldsymbol{c}_{N_t 1} & \cdots & \boldsymbol{c}_{N_t|\mathcal{E}|} \end{bmatrix} \begin{bmatrix} \xi_1 \\ \vdots \\ \xi_{|\mathcal{E}|} \end{bmatrix} = \begin{bmatrix} \sum_{e\in\mathcal{E}} \boldsymbol{c}_{1e} \\ \vdots \\ \sum_{e\in\mathcal{E}} \boldsymbol{c}_{N_t e} \end{bmatrix} \quad \rightarrow \quad \boldsymbol{C}\boldsymbol{\xi} = \boldsymbol{d}$$

Exact assembly satisfies $C1 = d$ $\quad\rightarrow\quad$ Find sparse set of weights s.t. $C\xi \approx d$

OPTIMAL SAMPLE WEIGHT COMPUTATION

- Computing the sample weights ξ_e via ***large-scale supervised learning***

$$\begin{aligned} \text{minimize} \quad & \|\boldsymbol{\xi}\|_0 \\ \text{subject to} \quad & \|\boldsymbol{C}\boldsymbol{\xi} - \boldsymbol{d}\|_2 \leq \varepsilon \|\boldsymbol{d}\|_2 \\ & \boldsymbol{\xi} \geq 0 \end{aligned}$$

  - ℓ^0-pseudonorm minimization is NP-hard and thus generally intractable

- Solve instead a convex approximation which promotes sparsity: non-negative least squares

$$\begin{aligned} \text{minimize} \quad & \|\boldsymbol{C}\boldsymbol{\xi} - \boldsymbol{d}\|_2 \\ \text{subject to} \quad & \boldsymbol{\xi} \geq 0 \end{aligned}$$

  equipped with an early termination criterion

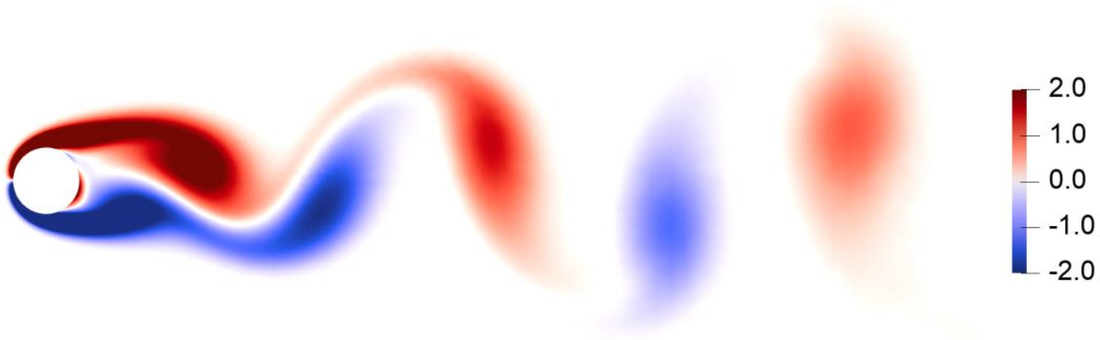
$$\|\boldsymbol{C}\boldsymbol{\xi} - \boldsymbol{d}\|_2 \leq \varepsilon \|\boldsymbol{d}\|_2$$

  - Significant work developing solvers to deal with large problem size (storage for $\boldsymbol{C}$ quickly exceeds 1TB for problems of interest)

Performance assessment for laminar and RANS flow models

2D LAMINAR FLOW OVER A CIRCULAR CYLINDER, REVISITED

- HDM characterization
  - Compressible Navier-Stokes equations semi-discretized using a second-order mixed FV/FE scheme
  - Implicit time discretization using second-order DIRK scheme
  - Resulting dimension $\boldsymbol{N}$ ***= 490,700***

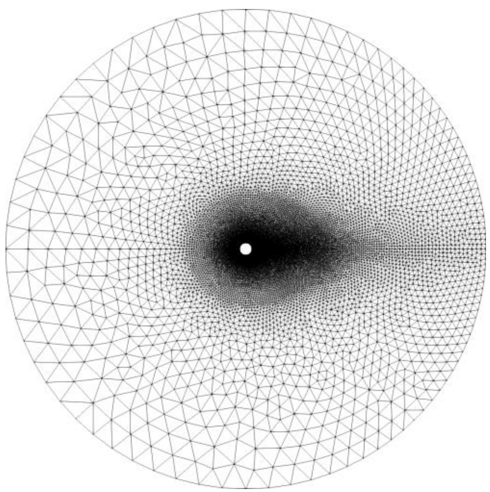


Solution vorticity snapshot

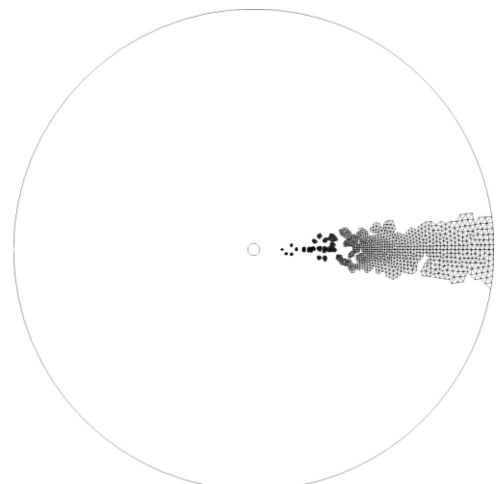
- Petrov-Galerkin PROM construction
  - Least-squares Petrov-Galerkin (LSPG) projection
  - 751 collected snapshots from $t \in [0, 150]$ yield ROB $\boldsymbol{V}$ of dimension $\boldsymbol{n}$ ***= 35*** using POD

2D LAMINAR FLOW OVER A CIRCULAR CYLINDER, REVISITED

- Hyperreduction training
  - Proposed ECSW adaptation with tolerance $\varepsilon = 0.01$ and 376 solution snapshots, taken as every second one used for POD
  - Mesh sampling yields $|\tilde{\mathcal{E}}| = 376$, sampled cells ***(0.33% of HDM mesh cells)***



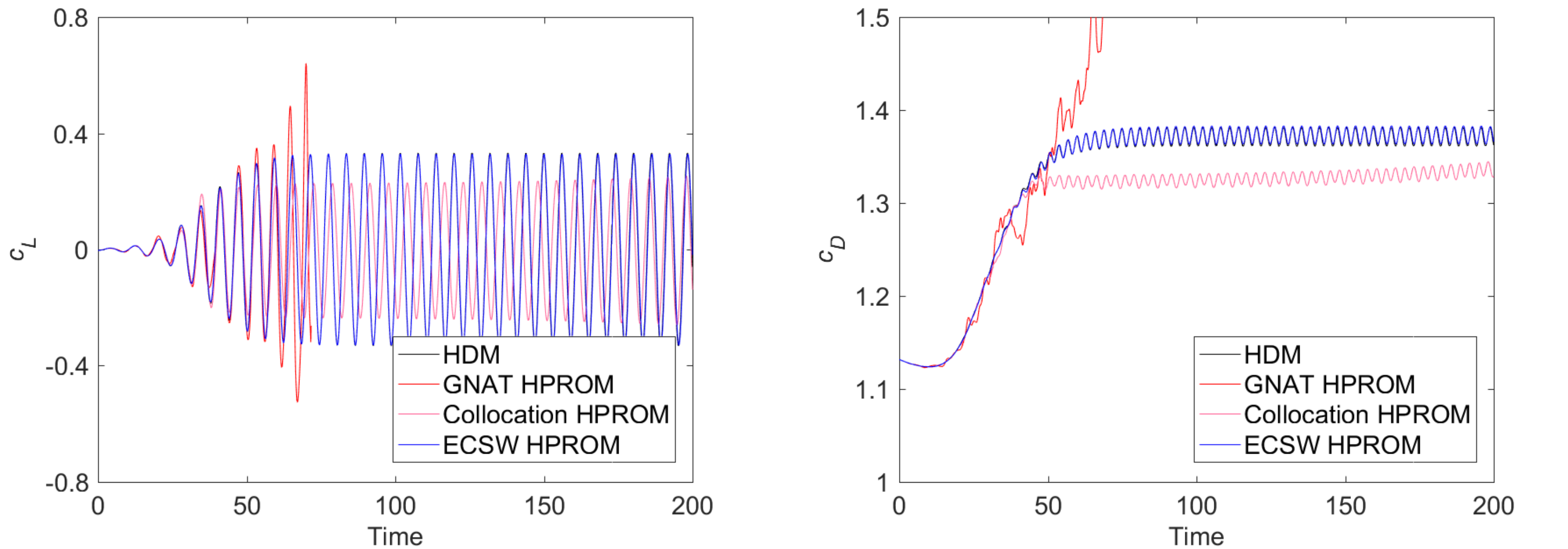
Original mesh



Reduced mesh

2D LAMINAR FLOW OVER A CIRCULAR CYLINDER, REVISITED

- Comparison of lift and drag coefficient time histories as computed by the HDM, ECSW-based hyperreduced PROM (HPROM), and two alternative state-of-the-art hyperreduction methods



- ECSW-based HPROMs are numerically stable and accurate, even outside of trained time interval when solution remains periodic
  - Results also hold for solution computed at probes instead of integrated quantities

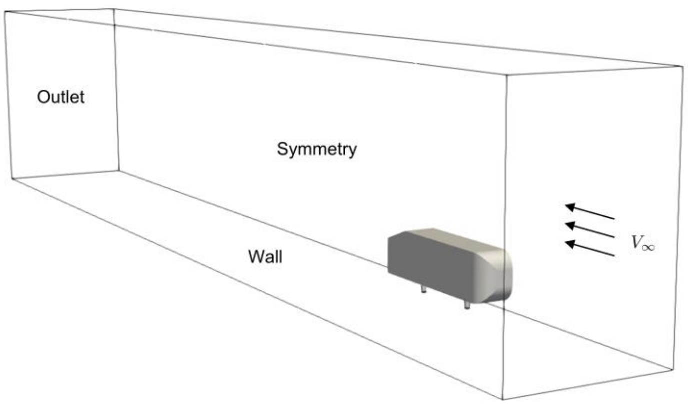
2D LAMINAR FLOW OVER A CIRCULAR CYLINDER, REVISITED

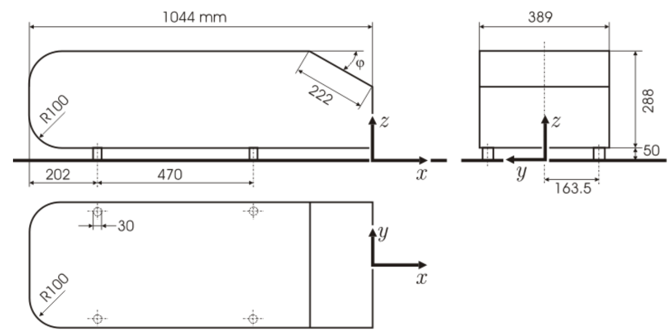
- Comparison of wall-clock times for HDM- and HPROM-based simulations (both performed on a single core)
  - HDM solution: 65.4 hours
  - HPROM solution: 2.8 minutes

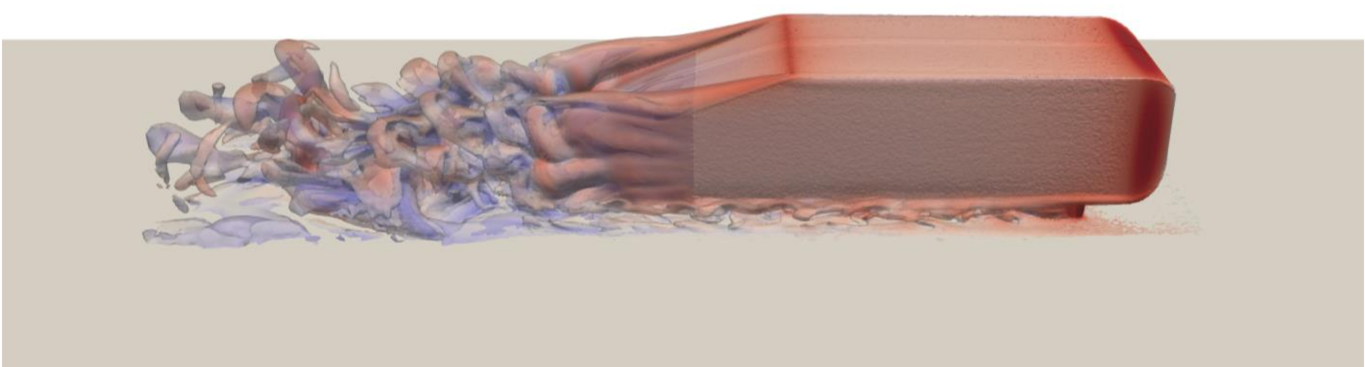
Wall-clock time speedup factor = 1,410

TURBULENT AHMED BODY WAKE FLOW

- Detached eddy simulation (DES) of flow past the Ahmed body geometry with slant angle = 20°
  - $Re = 4.29 \times 10^6$, $V_\infty = 60$ m/s
  - Common benchmark problem in the automotive industry





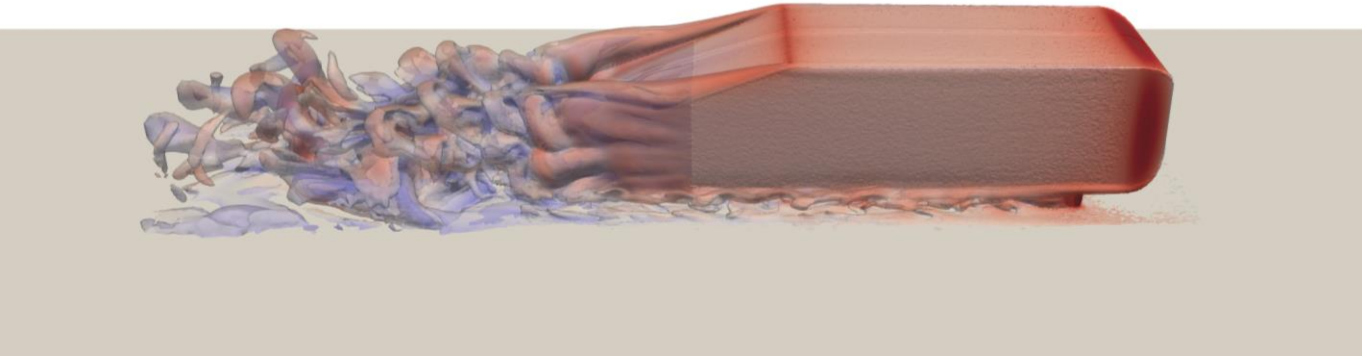


Contours of vorticity magnitude colored by Mach number

TURBULENT AHMED BODY WAKE FLOW

- HDM, PMOR, and hyperreduction
  - Computational domain discretized using 2.9M vertices and 17.0M tetrahedra, leads to HDM dimension $\boldsymbol{N = 17{,}342{,}604}$
  - *Local* subspace approximations are constructed with average dimension $\boldsymbol{\bar{n} = 86, 29,}$ and ***11*** (corresponding to 10, 50, and 100 local subspaces)
  - Sampled cells for ECSW-based HPROMs:

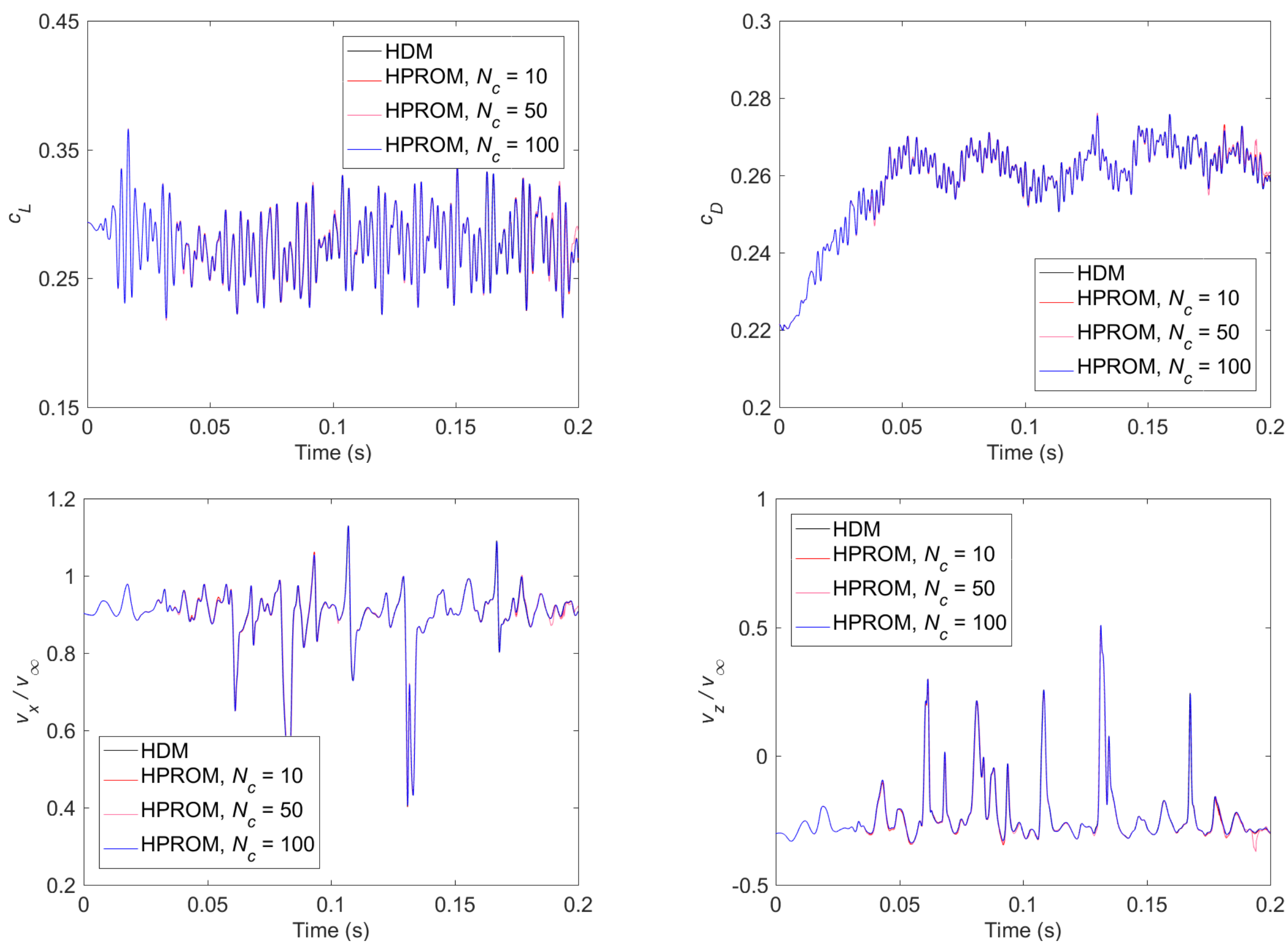
# of subspaces	$\lvert\tilde{\mathcal{E}}\rvert$	$\lvert\tilde{\mathcal{E}}\rvert/\lvert\mathcal{E}\rvert$
10	1,620	**0.056%**
50	347	**0.012%**
100	137	**0.0047%**



Contours of vorticity magnitude colored by Mach number

TURBULENT AHMED BODY WAKE FLOW

- Comparison of lift and drag coefficient time histories and velocity computed at a probe using the HDM and each local HPROM
  - Probe is located 0.5 body lengths downstream in wake



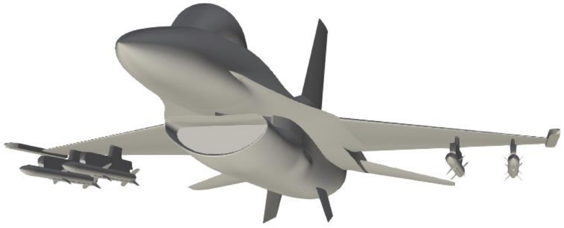
TURBULENT AHMED BODY WAKE FLOW

- Comparison of wall-clock times for HDM- and HPROM-based simulations
  - HDM solution computed on 240 cores
  - HPROM solutions computed on 8 cores

Model	*# of subspaces*	*Wall-clock time*	*Wall-clock time speedup factor*	*CPU time speedup factor*
HDM	-	12.1 hours	-	-
	10	10.4 min	**70**	**2,090**
HPROM	50	1.3 min	**572**	**17,200**
	100	36.8 s	**1,190**	**35,600**

TURBULENT FLOW PAST AN F-16C/D FIGHTER JET

- Unsteady flow simulation past an F-16C/D fighter jet model at 30° angle of attack
  - Freestream conditions: 10,000 ft altitude, M_∞ = 0.3, Re = 18.2 × 10^6
  - Complex geometry and high angle of attack results in massive flow separation and formation of turbulent vortical structures



- High-fidelity, high-dimensional flow model
  - Compressible Navier-Stokes equations, one-equation RANS turbulence model
  - Unstructured tetrahedral mesh with 26.9M vertices and 159.0M elements, resulting dimension $\boldsymbol{N}$ = **161.5M**
  - Second-order implicit time integration, 100,000 time steps for ∼1.3 s of physical time

TURBULENT FLOW PAST AN F-16C/D FIGHTER JET

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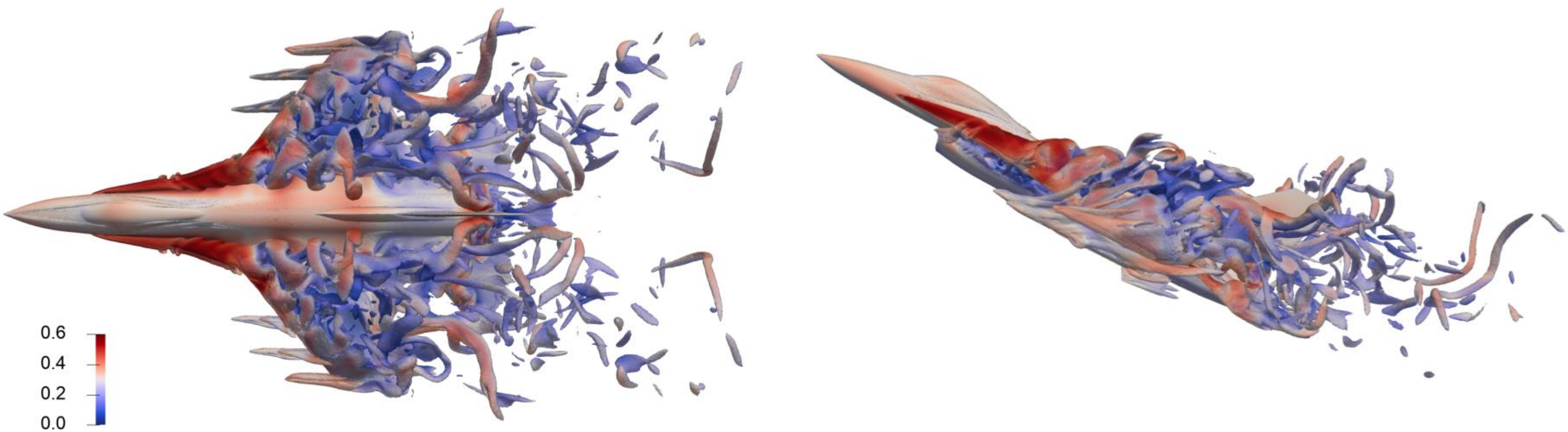


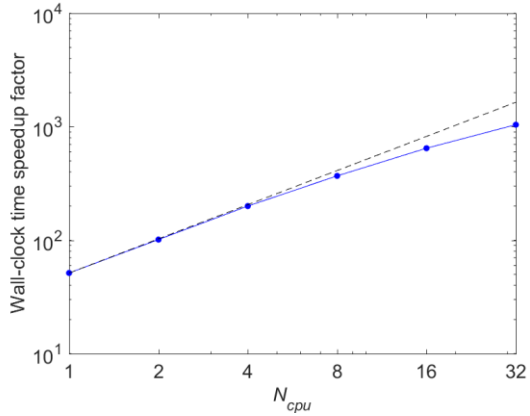
Contours of vorticity magnitude colored by Mach number

- Computational cost
  - Solution for time interval of interest ***requires 100.3 hours wall-clock time (~4 days) on 3,584 cores***

TURBULENT FLOW PAST AN F-16C/D FIGHTER JET

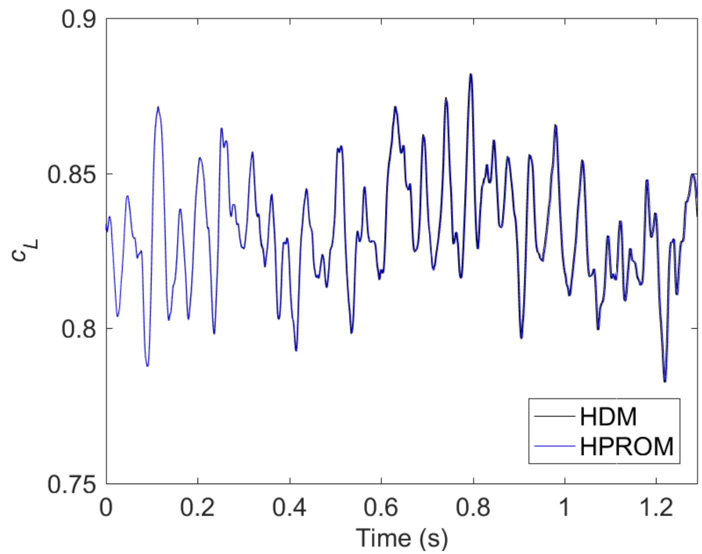
- Unsteady, nonparametric PMOR
  - Collect 5001 snapshots from the HDM simulation (every 20 time steps) and construct local subspace approximation with average dimension $\bar{n}$ ***= 53***
  - Hyperreduction training with error tolerance $\varepsilon = 0.01$ yields $|\tilde{\mathcal{E}}| = 787$ (vs. $|\mathcal{E}| = 26.9\text{M}$ $\rightarrow$ ***0.0029% of HDM mesh cells)***
  - Total training cost for subspace approximation & mesh sampling: 2.1 hours on 3,584 cores

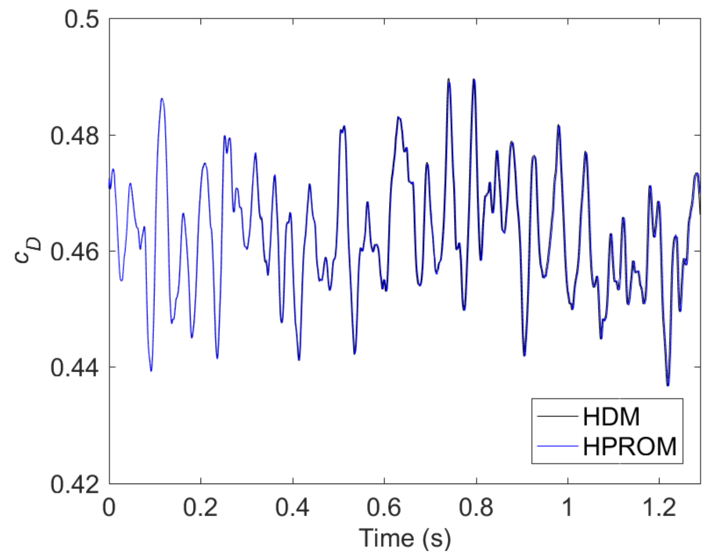
- HPROM-based simulation performance
  - ***5.8 minutes on 32 cores*** $\rightarrow$ wall-clock time speedup factor = 1,040
    CPU-time speedup factor = 117,000



TURBULENT FLOW PAST AN F-16C/D FIGHTER JET

- Comparison of lift and drag coefficient time histories computed by the HDM and HPROM

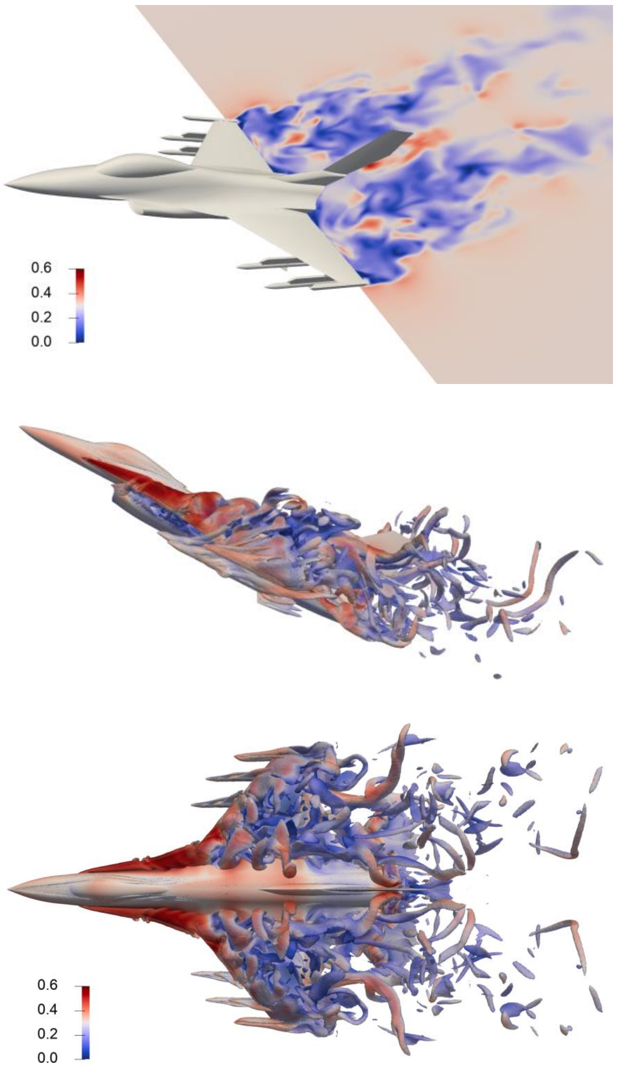




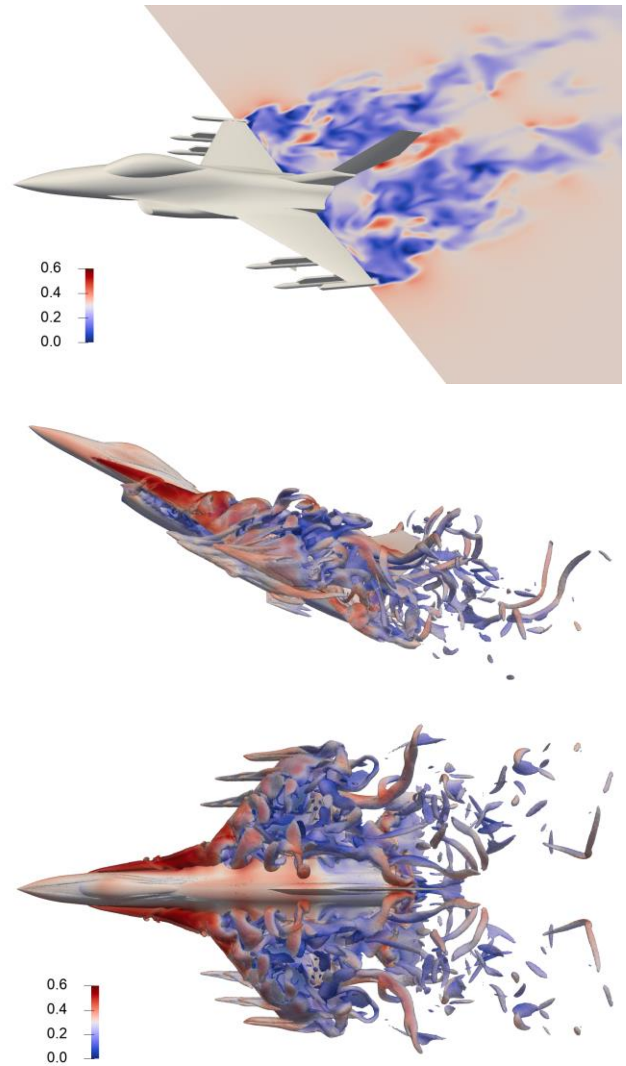
- ECSW-based HPROM captures with a high-degree of accuracy the HDM solution for time interval of interest

TURBULENT FLOW PAST AN F-16C/D FIGHTER JET

HDM



HPROM



SUMMARY AND CONCLUSIONS, PART II

- A new hyperreduction method for Petrov-Galerkin PROMs demonstrated to:
  - Outperform state-of-the-art methods for CFD models
  - Produce HPROMs for large-scale unsteady RANS-based CFD models which are both accurate and deliver large speedup factors

SUMMARY AND CONCLUSIONS

- Low-dimensional PMOR for convection-dominated and scale-resolving turbulent flow models is possible after making sure to take care of stability via the numerics

- Empirical quadrature via the ECSW method provides a practical and feasible hyperreduction framework for general nonlinear problems

- Perspectives for future work:
  - Time-dependent, parametric demonstrations with greedy adaptive parameter sampling
  - Nonlinear multiphysics applications: coupled fluid-structure interaction and embedded boundary methods